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The combustion model including aluminum and iron oxide was employed to correlate data bases of Miller and Maykut. Results for additive free formulations were excellent for both rate and exponent; results for formulations with aluminum and aluminum plus iron oxide were poor. A new method for extracting particle size dependent information from rate/response function/formulation data was developed from the statistical methodology itself and employed to process the aforementioned data bases. Results were encouraging; Miller's additive free and aluminum plus iron oxide data correlated very well; Millers aluminum data showed

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STATISTICAL ANALYSIS OF STEADY STATE COMBUSTION OF NONMETALLIZED COMPOSITE SOLID PROPELLANTS

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REPORT, CONTRACT F49620-76-C-0008

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BOLLING AIR FORCE BASE, D. C. 20332

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FOREWORD

This is a [redacted] report covering the work completed under Contract F49620-76-C-0008 for the period 1 July 1976 through 30 September 1977. Publication of this report does not constitute Air Force approval of the findings or conclusions contained herein. It is published only for the exchange of data and stimulation of ideas.

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ABSTRACT

The combustion model including aluminum and iron oxide was employed to correlate data bases of Miller and Maykut. Results for additive free formulations were excellent for both rate and exponent; results for formulations with aluminum and aluminum plus iron oxide were poor. A new method for extracting particle size dependent information from rate/response function/formulation data was developed from the statistical methodology itself and employed to process the aforementioned data bases. Results were encouraging; Miller's additive free and aluminum plus iron oxide data correlated very well; Miller's aluminum data showed that increasing aluminum particle size increases interactions among oxidizer modes; Maykut's data base showed that aluminum induced interactions among oxidizer modes are decreased as iron content increases. Results elucidate mechanisms for rate, exponent, and response function control and show that the equal rate hypothesis employed in much combustion modeling is incorrect. A new approach for including the effects of transients introduced by particle size dependent rates in both steady and nonsteady combustion modeling was conceived.

Goals of embedding Williams/Guirao AP decomposition model and Cohen nitramine model in the combustion model were not reached.

INTRODUCTION

Increasing emphasis on low visible exhaust signature in tactical applications of solid rocket motors has virtually eliminated significant amounts of condensed phases from the products of combustion. This has created a number of problems.

1. At equal total solids contents replacement of metal additive with AP reduces specific impulse.

2. Replacement of metal additive with oxidizer alters the relationship among rate, formulation, and environment.

3. Replacement of metal additive with oxidizer increases the probability of combustion instability because particle damping is absent.

The upshot is that propellant formulation is more difficult in the low signature area; all constraints imposed on a high signature formulation must be met at a higher total solids loading (if equivalent energetics are demanded) with greatly enhanced probability of combustion instability plus a new constraint-signature.

Propellant formulation has long proceeded in largely empirical channels. However, deviations of low signature formulations from the rate/formulation/environment relations established largely for metallized propellants over the past two decades, introduction of ingredients outside the historical data base (nitramines, ultra fine aluminum oxide, etc), and the importance of combustion instability have all contributed to increasing cost and risk of low signature propellant development efforts relative to those for similar high signature propellants. The economics of an empirical approach are strongly related to the cost of gathering data. With high signature systems only passing attention was paid to combustion stability; this is not the case for low signature systems. As a result, determination of propellant properties related to combustion stability accounts for a substantial portion of the aforementioned cost/risk differential.

Theory(1) shows that steady and nonsteady combustion phenomena are related for homogeneous propellants when the frequency is not too high. On phenomenological grounds a steady/nonsteady relation must also exist for composite propellants. However, it is not that for homogeneous propellants.(2) Since a steady/nonsteady relation means that propellant stability properties can be computed from steady-state data, it would be of considerable economic importance for low signature composite propellant development programs. Unfortunately, the empirical path followed by propellant developers virtually prohibits any possibility for discerning the aforementioned steady/nonsteady relation.

The overall objective of this work is to construct an analytical model describing steady-state combustion of composite propellants. This is both a worthy goal in itself (propellant constraints relate to steady-state properties) and a necessary step to understanding nonsteady phenomena.

TECHNICAL DISCUSSION

Combustion Modeling

Reference 3 presents mathematical developments for a steady-state combustion model of composite propellant with additives. Basically, a statistical procedure is employed to account for oxidizer particle size and additives are divided into either active or passive categories. In the former category, the additive modifies the kinetics of the deflagration process; in the latter the additive acts solely as an inert heat sink. In this program this model has been transformed into an operational computer code and employed to correlate experimental data.

The data bases of Miller[4] and Maykut[5] have been employed to test the model. Miller's data base includes additive free, aluminum additive, and aluminum plus iron oxide additives. Maykut's data base includes aluminum and varying amounts of iron oxide. Both data bases are for HTPB/AP formulations and have similar total solids contents.

The correlation process proceeded as follows. First, basic parameters were adjusted to give a "best" fit with Miller's additive free data. Second, with these parameters, rates and exponents were predicted for Miller's 24 micron aluminum additive formulations (no additional parameters are required to account for passive additives). Third, parameters associated with the iron oxide catalyst were adjusted to give a best fit to selected rate vs catalyst data in Maykut's data base. Fourth, rates and exponents were predicted for the formulations in Miller's 24μ aluminum plus 1% iron oxide data base and the remainder of Maykut's data base.

Results for Miller's additive free data are reported elsewhere.[6] The correlation was superb for both rate and exponent. The standard error of estimate of the correlation was roughly 6 percent. This is of the same order as errors in the burning rate measurements themselves. Consequently, the correlation is essentially as good as the data itself.

Figures 1 and 2 present the correlation of Miller's 24 micron aluminum data (formulation set SD-I-88). It is clear that appreciable scatter exists. Examination of the outlyers* shows that, in general, they are formulations possessing a "wide" distribution. Consequently, the present model seems adequate only for metallized propellants with narrow distributions. As Miller has pointed out elsewhere[7], the addition of aluminum causes interactions to occur among particles of differing size. As presently constituted, the combustion model does not include interactions.

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*Numbers associated with the formulations are the formulation numbers assigned by Miller.[4]

Figures 3 and 4 present the correlation of Miller's 24 micron aluminum plus 1% iron oxide data (formulation set SD-VII-88). There is considerable scatter in this correlation. However, when contrasted with the aforementioned aluminum additive data the scatter does not appear to relate to wide and narrow distributions. Indeed, it appears that there is a systematic error in the predicted exponents (refer to the dashed correlation line) and that propellants with rates below 1 in/sec systematically deviate from the above 1 in/sec correlation. The latter behavior was evident in correlations of the same data presented by Beckstead.[8]

Figures 5 and 6 present the correlation of Maykut's HTPB/AP/30μ Al/ iron oxide data base. As before, there is appreciable scatter. However, the character of the scatter differs from that of Miller's 24μ Al plus iron oxide data base. Here the outlyers are largely those with wide distributions. Moreover, the rate correlation possesses a systematic deviation (dashed line) while the exponent correlation doesn't.

In summary, correlation of these systematic data bases has shown that the basic additive free model appears to be adequate while the model for additives is inadequate. It is clear that metal additives cannot be treated as simple heat sinks. However, problems with the present treatment of catalysts are confounded with aluminum effects. An extensive catalyst data base without metal additive is required to adequately define inadequacies in the catalyst model.

Analysis of Data With the Statistical Framework

The aforementioned results show that the present combustion model is, at present, inadequate for quantitative calculations with propellants containing additives. In the combustion model errors can arise from two sources (a) the statistical framework and (b) the unit combustion model. One suspects that the statistical framework is more accurate than the unit combustion model. Therefore, effort was expended to explore use of the basic statistical framework to correlate data.

Correlation of Miller's additive free data had shown that best correlation occurs when the pseudo-propellant oxidizer/fuel ratios are all equal. Thus, $\alpha^*_{ox,k} = \alpha_{ox}$ so that the basic rate equation

$$\bar{m}_t = \oint_D (\bar{m}_D / \alpha^*_{ox,k}) \sum_{k=1}^{M} \alpha_{ox,k} F_{ox,k} \, dD/D \tag{1}$$

becomes

$$\bar{m}_t = \alpha_{ox}^{-1} \sum_{k=1}^{M} \alpha_{ox,k} \oint_D \bar{m}_D F_{ox,k} \, dD/D \tag{2}$$

The integral in the latter equation is the mean mass flux from the pseudo-propellant containing the kth oxidizer mode. Therefore, Eq. (2) can be rewritten as

$$\overline{m}_t = \alpha_{ox}^{-1} \sum_{k=1}^{M} \alpha_{ox,k}\, \overline{m}_k \tag{3}$$

which leads to

$$\overline{r}_t = \alpha_{ox}^{-1} \sum_{k=1}^{M} \alpha_{ox,k}\, \overline{r}_k \tag{4}$$

since $\alpha^{*}_{ox,\Delta} = \alpha_{ox}$. Differentiation of Eq. (4) leads to

$$d\overline{r}_t = \alpha_{ox}^{-1} \sum_{k=1}^{M} \alpha_{ox,k}\, \overline{r}_k \, d\overline{r}_k / \overline{r}_k \tag{5}$$

Therefore, algebraic manipulation yields

$$\overline{n}_t = (\alpha_{ox}\, \overline{r}_t)^{-1} \sum_{k=1}^{M} \alpha_{ox,k}\, \overline{r}_k\, \overline{n}_k \tag{6}$$

$$\overline{\sigma}_{p,t} = (\alpha_{ox}\, \overline{r}_t)^{-1} \sum_{k=1}^{M} \alpha_{ox,k}\, \overline{r}_k\, \overline{\sigma}_{p,k} \tag{7}$$

$$\overline{R}_{p,t} = (\alpha_{ox}\, \overline{r}_t)^{-1} \sum_{k=1}^{M} \alpha_{ox,k}\, \overline{r}_k\, \overline{R}_{p,k} \tag{8}$$

These equations assert that the ballistic properties of composite propellants should be expressible in terms of modal properties. On the other hand, experimental data can be analyzed to determine these modal properties. That is, if ballistic data from at least N formulations with the same chemical composition but differing median oxidizer size were available, the $\overline{r}_k$, $\overline{n}_k$, etc ($k = 1, N$) could be computed from that data. Once these $\overline{r}_k$, $\overline{n}_k$, etc ($k = 1, N$) were known, the ballistic properties of <u>any</u> formulation with that chemical composition could be computed. Consequently, ballistic properties of all members of a bimodal family with fixed chemical composition but differing particle size could be defined from ballistic data for just two members; a trimodal family would require data from three members.

In short, it appears that the statistical framework offers some exciting possibilities for generalizing experimental ballistic data. In addition, the modal pseudo-propellant properties demonstrate the effects of particle size and additives at a level much closer to the unit combustion model. Therefore, the "statistical framework approach" also offers some exciting possibilities for assisting the theoretical modeling.

To test the "accuracy" of the statistical framework for correlating ballistic data a computer code for extracting the best, in a statistical sense,

$\overline{r}_k, \overline{n}_k$ from any data set was developed. Appendix B presents the code and a sample case illustrating input and output. Figures 7 and 8 present the correlation of Miller's additive free rate and pressure exponent data while Table 1 presents the best fit $\overline{r}_k$ and $\overline{n}_k$. Correlation in all cases is superb.

Figures 9 and 10 present the correlation of Miller's 24 micron aluminized propellant data while Table 1 presents the best fit $\overline{r}_k$ and $\overline{n}_k$. The presence of of aluminum degrades the correlation. However, data scatter is much less than that shown by Figures 1 and 2. Therefore, an appreciable portion of the inaccuracy in the theoretical model must be attributable to the unit combustion model. It is important to note that the data outlyers are generally associated with formulations possessing wide oxidizer distributions. Consequently, there is every reason to believe that if interaction effects were included in the statistical framework the outlyers would be brought into the fold.

Figures 11 to 14 present correlations for Miller's 6 micron and 90 micron aluminized propellant data while Table 1 presents the best fit $\overline{r}_k$ and $\overline{n}_k$. Comments pertinent to the individual data correlation are essentially the same as those for the 24 micron data. However, when Figures 9, 11, and 13 are viewed in sequence it is obvious that the correlation degrades with increasing aluminum particle size. This trend is also evident in the standard error of estimate data of Table 1. Thus, interaction effects must increase with increasing aluminum particle size.

Figures 15 and 16 present correlations for Miller's 24 micron plus 1 percent iron oxide propellant data while Table 1 presents the best fit $\overline{r}_k$ and $\overline{n}_k$. Correlation of this data is superb. Clearly, as Miller has noted, the addition of 1% iron oxide has suppressed (or compensated for) interactions among the oxidizer particles.

Table II presents modal rates and exponents and statistical measures of the correlation of Maykut's data base. Several trends are noted. First, the correlation improves as pressure decreases. This suggests that interactions are related to transport property effects since kinetics become of increasing importance as pressure decreases. Second, the correlation improves as catalyst content increases. This shows that catalyst progressively cancels (or compensates) interactions. Note that in Miller's data 1% catalyst eliminated interactions while 2% catalyst is required here. Third, note that catalyst has little effect on the 16μ mode; effects appear to be concentrated in the coarse and fine modes.

The above results show that the correlation methodology possesses excellent capabilities for extracting modal properties under circumstances when interactions are small. Data from these situations may be employed to elucidate particle dependent combustion phenomena. Figure 19 presents the variation of modal burning rate with volume mean particle size for Miller's additive free formulations. It is clear that burning rate depends strongly upon oxidizer particle size and that variation is pressure dependent. Note that at 500 psi there is little variation of rate with particle size for particles below 10μ. This indicates that small particle rates are kinetic rather than diffusion limited. Note that this situation alters as pressure increases. Figure 20 compares the diametral dependence of burning rate with formulation for Miller's data base. The addition of aluminum substantially degrades the burning rates of fine material while producing relatively little effect on the coarse modes. The addition of catalyst causes substantial increases in the burning rate of both fine and coarse AP modes but little effect in the 50 to 100μ range. Figure 21 illustrates the dependence of modal exponent on volume mean diameter of the mode for several formulations in Miller's data base. For the additive free formulation exponent increases to unity as diameter decreases. This indicates that as diameter approaches zero rate control shifts to a kinetic mechanism. The surprising result is the tendency for exponent to increase for very coarse oxidizer modes. The mechanism for this increase is not known. However, the combustion model predicts this trend.[6] The effect of both aluminum and catalyst is primarily to suppress high exponents at small particle sizes.

The modal property trends shown in Figures 20 and 21 explain many formulation trends. For example, rate is sensitive to the amount of coarse material because rate is weighted solely by mass fraction. However, exponent is much less sensitive to the amount of coarse material because the exponent is weighted by both mass fraction and rate and the modal rates of coarse material are low. Thus, rate tends to be controlled by both coarse and fine while exponent is largely controlled by the fine fraction. With the data in hand it is clear that high exponent ($n > 0.7$) formulations with significant metal content are highly improbable in a HTPB/AP/Al/Iron Oxide system; the modal exponents are all low. On the other hand, high exponent can be readily achieved in an additive free system simply by incorporating small diameter fines.

It appears that inert additives act to suppress both rate and exponent of fine AP. Rate can be restored with a catalytic additive, but exponent apparently cannot. This suggests that inert additives should provide means for reducing exponent independent of particle size control while a mixture of inert/catalytic additives should provide means for controlling both rate and exponent independent of particle size control.

The functional similarity of Eqs. 6 and 8 and the fact that $\overline{R}_{p,t}$ approaches $\overline{n}_t$ as frequency approaches zero suggests strongly that techniques for exponent control should carry over into control of pressure coupled response. From the arguments presented above it is seen that propellants formulated with significant amounts of coarse AP should possess both low exponent and low pressure coupled driving. Moreover, inert additives should be excellent stability additives. These trends have substantially been borne out.[10] The efficacy of inert additives has generally been laid at the doorstep of particle damping. However, the above suggests that part of the observed effects may be attributed to reduced pressure coupled driving.

It is important to note that the R_p, n "analogy" is definitely not exact. The reason is that the frequency where the response function peaks varies with the thickness of the subsurface energy store which varies locally with rate. What this means is that dynamic effects cloud the issue. Therefore, the above formulation generalizations will probably vary with frequency.

It is unfortunate that available data bases do not usually contain either temperature sensitivity or response function information (Miller's data base will eventually supply limited response function information). Without systematic data in these areas we are simply working in the dark.

Strategy for Inclusion of Nonsteady Phenomena in Combustion Modeling

Combustion phenomena in composite propellants is inherently nonsteady at the single particle level. That is, even when the environment is quiescent $r = r(x,t)$ where x denotes position on the burning surface. This, in turn, implies that $T_s = T_s(x,t)$ and $q''_{\bar{s}} = q''_{\bar{s}}(x,t)$. However, all steady-state combustion models are functionally equivalent to the assumption that $q''_{\bar{s}}$ and T_s are not functions of time. This is justified by assuming that transient phenomena cancels in the summation to a mean state. If the mean state is to be one of the accessible physical states, this assumption is generally false; the magnitude of the error introduced by this assumption is unknown.

The success of the steady-state models in dealing with Miller's additive free formulations suggests (but does not prove) that when the environment is quiescent these errors are small. However, in models that employ the equal rate hypothesis $r(D) = r(D+\Delta D)$ surface temperature, subsurface energy store, and surface heat flux are equivalent for all particles. Consequently, for low and midfrequency response where the chemically reactive zones behave quasi-steadily, the response function should possess characteristics similar to those of a homogeneous propellant (single relative maximum). On the other hand, if $r(D) \neq r(D + \Delta D)$ surface temperature and heat flux are not unique. Therefore, the possibility of a multi-relative maximum response function exists. The factor that distinguishes among these possibilities is the subsurface temperature profile.

In existing nonsteady models approximations have been introduced. Condon and Glick[2] have assumed that each monodisperse pseudo-propellant in the set representing the composite propellant possesses its equilibrium subsurface temperature profile. Cohen[9] has introduced the particle diameter as a length scale and thereby assumed the characteristic thermal thickness is proportional to particle size. Results depend strongly upon these assumptions.[2]

The major difficulty with current approaches to the condensed phase heat transfer aspects of the composite propellant combustion problem is that they are deterministic when the physical problem has a probabilistic character. For steady-state probabilistic phenomena probabilities in the spatial domain at fixed time are equivalent to probabilities in the temporal domain at fixed spatial coordinates. Thus, in a one-dimensional sense the propellant can be viewed as a super Dagwood sandwich of the monodisperse pseudo-propellants (refer to Figure 22). As the monodisperse pseudo-propellants all possess the same bulk thermal properties <u>in the mean</u>, these properties are common to the sandwich layers. Therefore, the temperature field is governed by

$$\partial T/\partial t = \kappa\, \partial^2 T/\partial y^2 - r\, \partial T/\partial y \tag{6}$$

The initial condition is clearly

$$T(-\infty, t) = T_0 \tag{7}$$

Following Z-N[1] appropriate boundary "conditions" that enable computation of r(t) are

$$r = r\,(q''_{\bar{s}},\ p, D) \tag{8}$$

$$T_s = T_s\,(q''_{\bar{s}},\ p, D) \tag{9}$$

$$p = p(t) \tag{10}$$

In conventional Z-N strategy r and T_s are not functions of particle diameter because conventional Z-N strategy applies solely to homogeneous propellants. Since deflagration occurs through a layered medium here the additional independent variable must occur.*

The Z-N boundary conditions can be derived from any steady-state source since the Z-N form of the boundary conditions is independent of time as long as the reactive regions are quasi-steady. The obvious source is from a detailed combustion model. However, by employing the aforementioned methodology to extract modal properties from experimental data a source much closer to basic experimental data <u>may</u> be available. The latter approach is in the original spirit of Z-N methodology which was aimed at circumventing need for combustion modeling.

The last question to be answered is how are the pseudo-propellant layers arranged. The answer of course is randomly such that the probability of finding pseudo-propellant with $D \leq D \leq D+dD$ is equivalent to the volume fraction of that pseudo-propellant in the propellant recipe. This is the probabilistic aspect of the problem.

The output of this approach for a small sinusoidal environment variation will be both the mean burning rate and the small signal response to that variation (pressure coupled response function). In addition, mean rates and small signal response functions for each pseudo-propellant should be recoverable.

*The methodology can also account for velocity coupling.[1]

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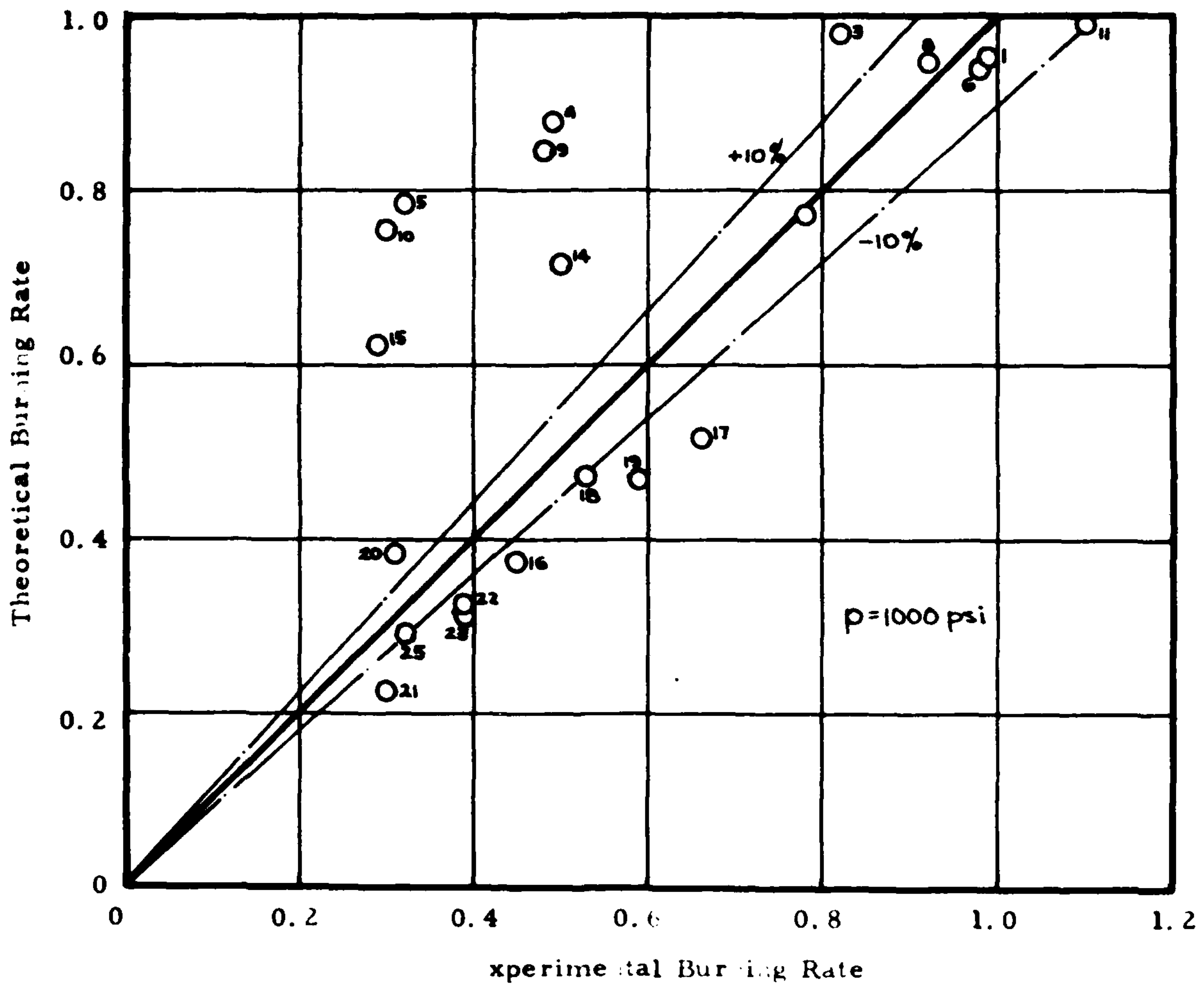

Figure 1. Burning Rate: Calculated versus Experimental for Miller's 24 micron Aluminum Additive Data Base (SD-I-88)

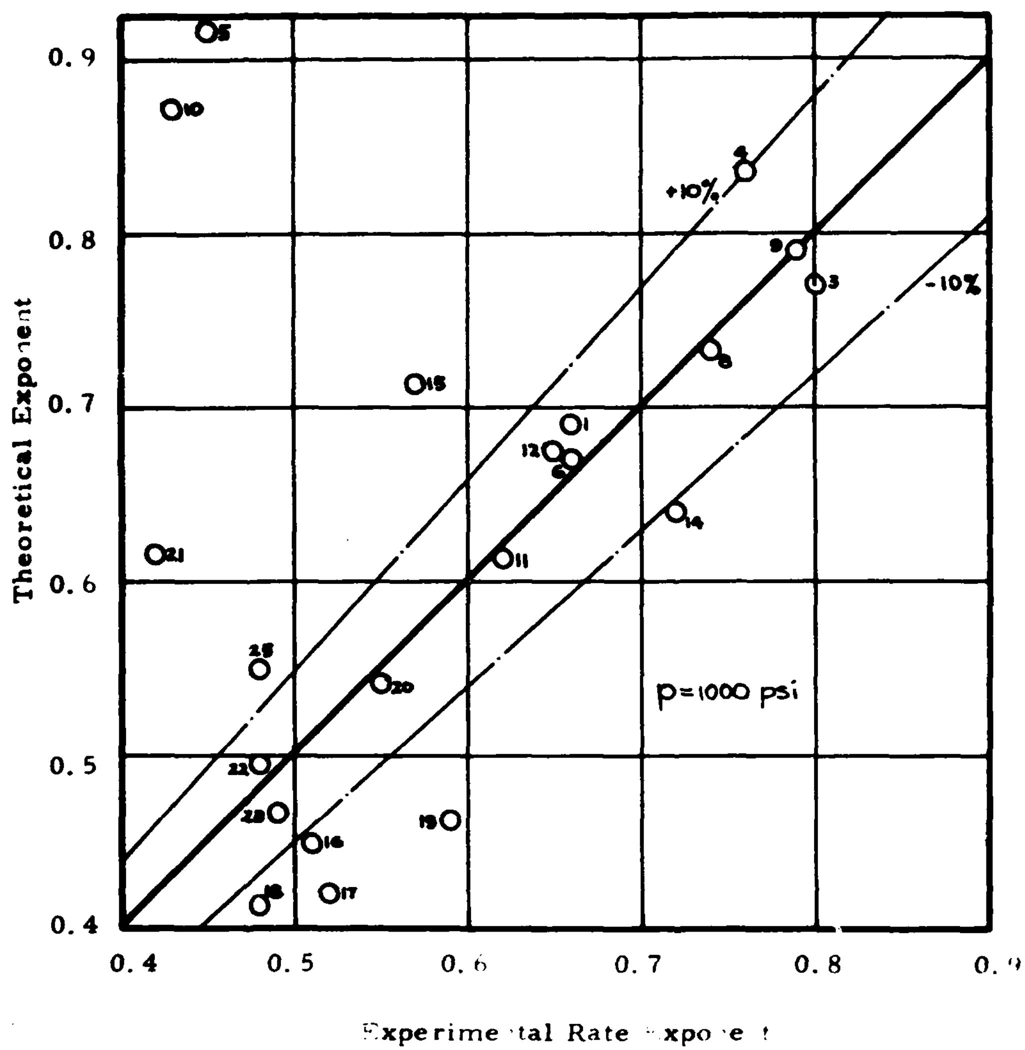

Figure 2. Burning Rate Exponent: Calculated versus Experimental for Miller's 24 micron Aluminum Additive Data Base (SD-I-88)

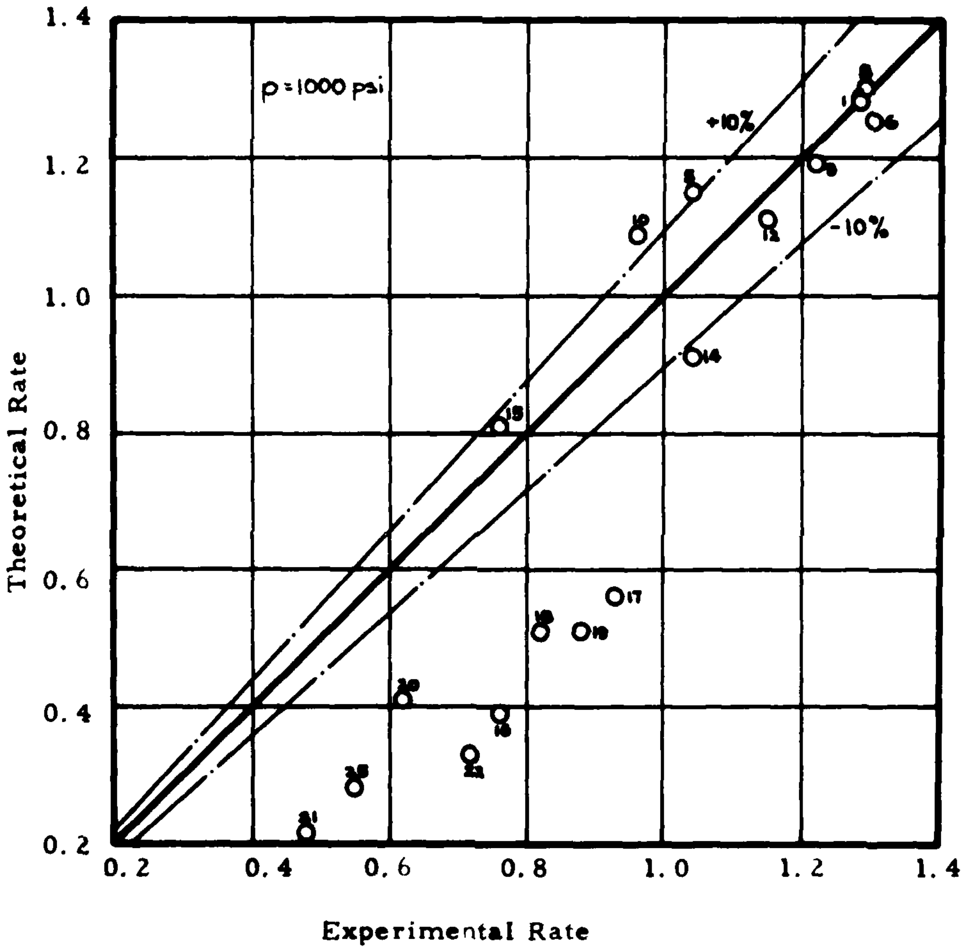

Figure 3. Burning Rate: Calculated versus Experimental for Miller's 24 micron Aluminum plus 1% Iron Oxide Data Base (SD-VII-88)

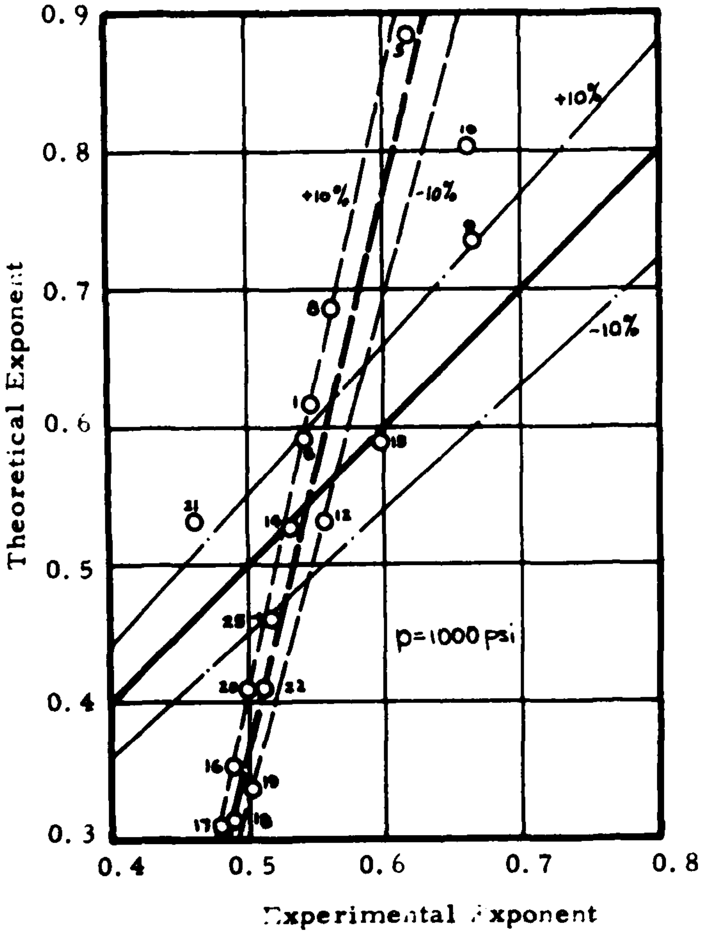

Figure 4. Burning Rate Exponent: Calculated versus Experimental for Miller's 24 micron plus 1% Iron Oxide Data Base (SD-VII-88)

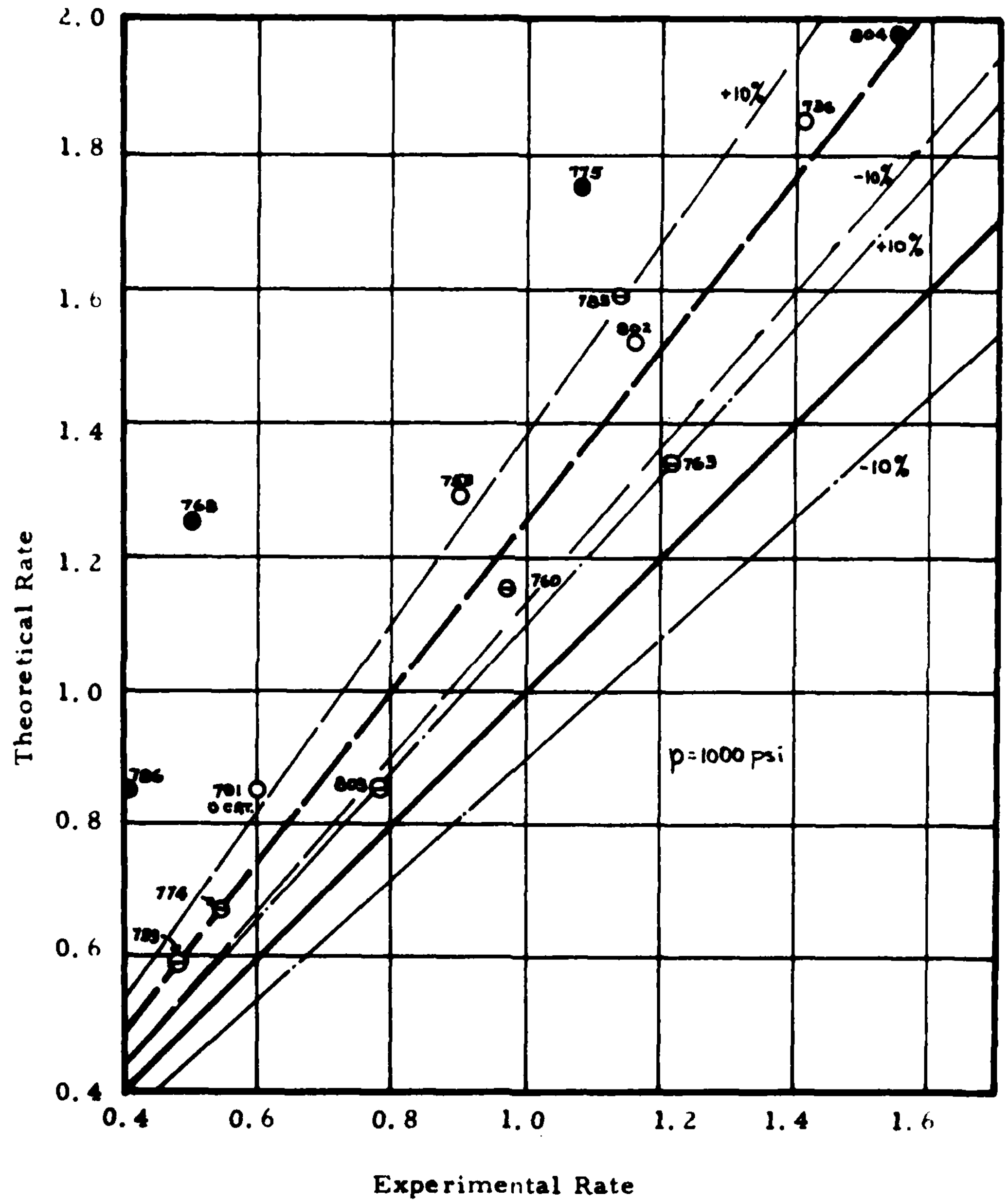

Figure 5. Burning Rate: Calculated versus Experimental for Maykut's Data Base

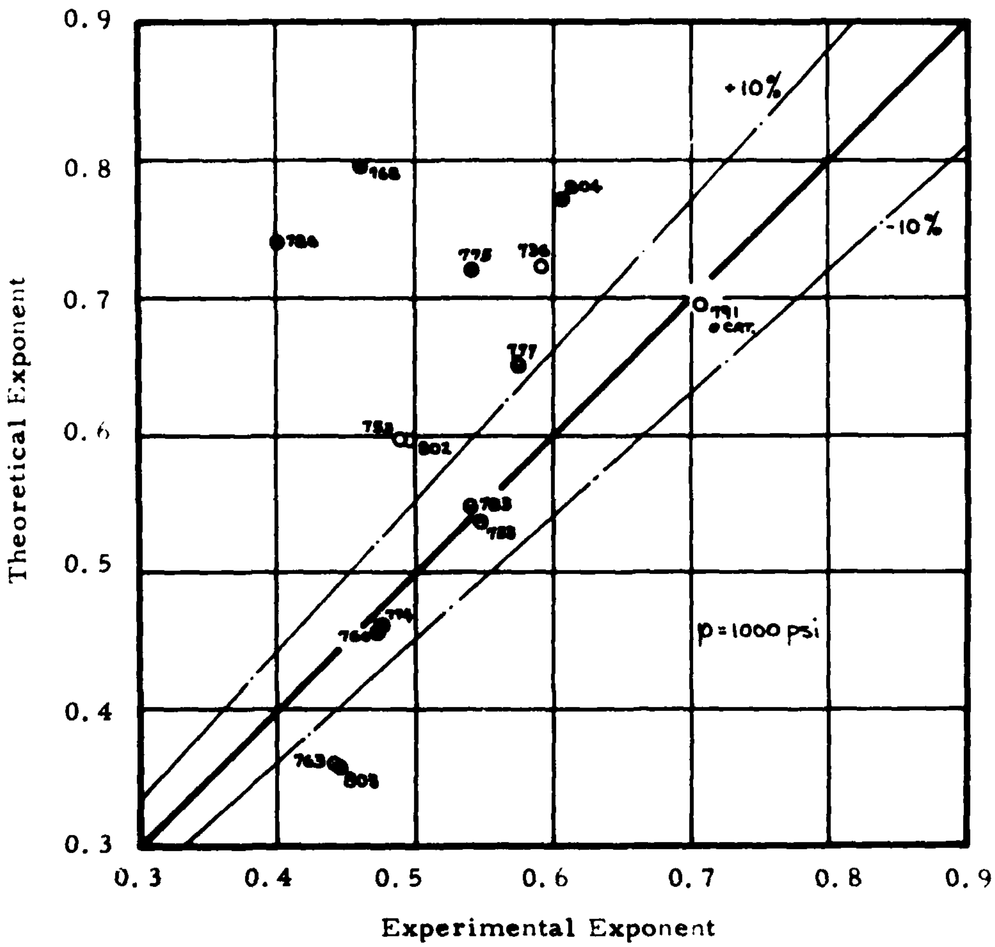

Figure 6. Burning Rate Exponent: Calculated versus Experimental for Maykut's Data Base

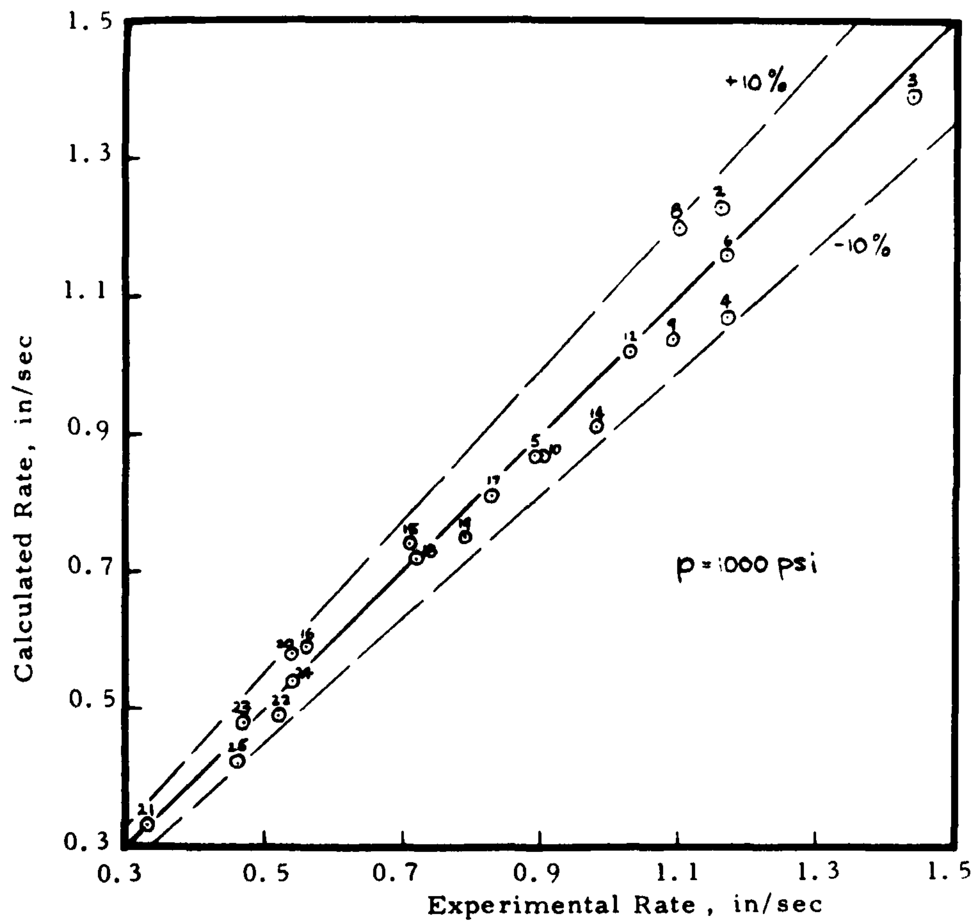

Figure 7. Burning Rate: Calculated versus Experimental for Miller's Additive Free Data Base (SD-III-88)

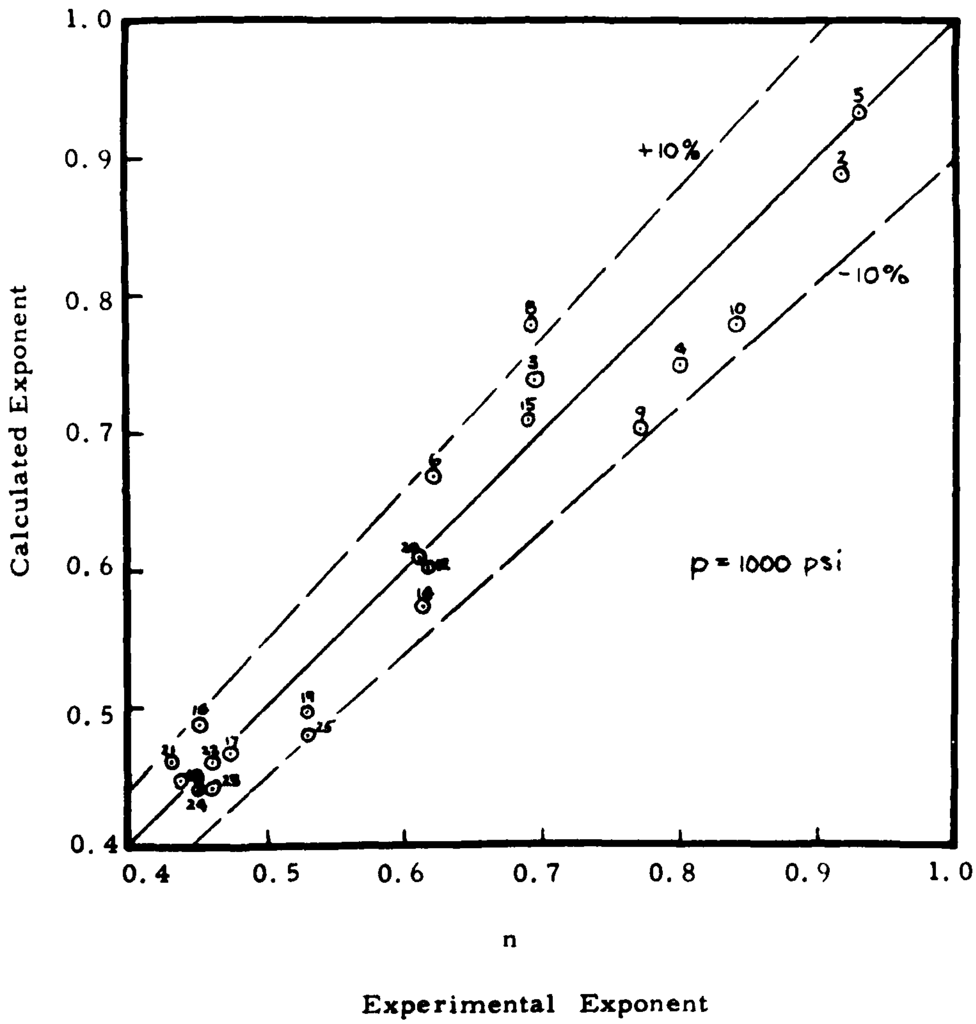

Figure 8. **Exponent: Calculated Versus Experimental for Miller's Additive Free Data Base (SD-III-88)**

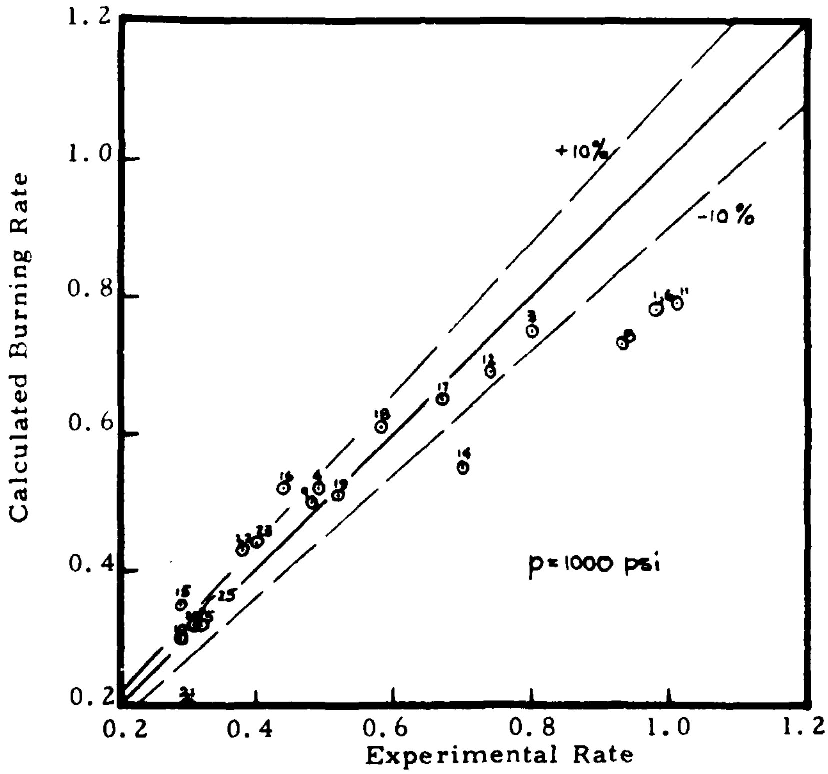

Figure 9. Burning Rate: Calculated versus Experimental for Miller's 18% 24-micron Aluminum Data Base (SD-I-88)

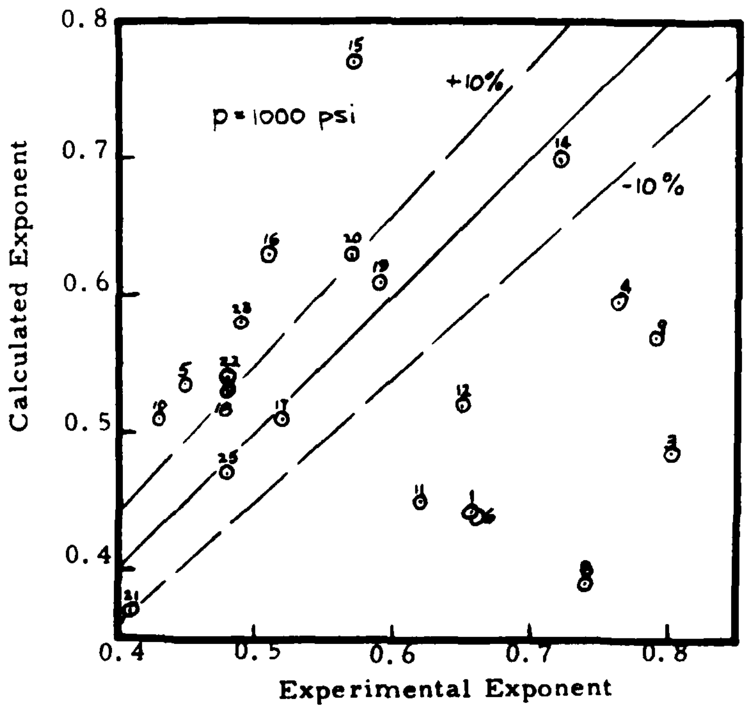

Figure 10. Burning Rate Exponent: Calculated versus Experimental for Miller's 24 micron Aluminum Additive Data Base (SD-I-88)

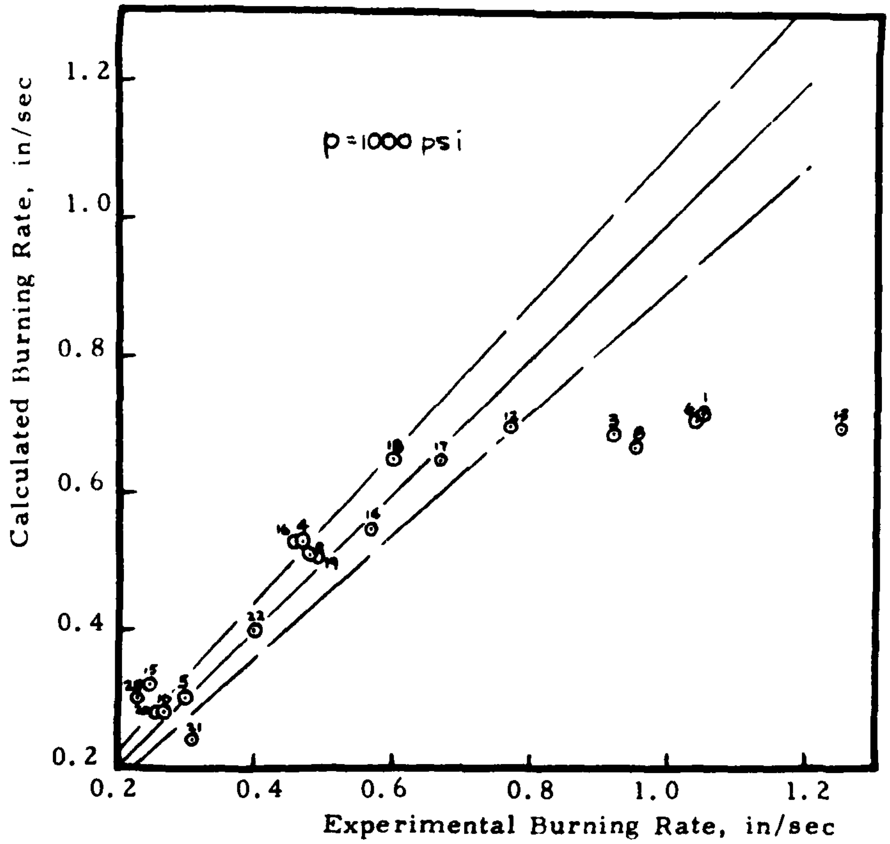

Figure 11. Burning Rate: Calculated versus Experimental for Miller's 90 micron Aluminum Additive Data Base (SD-IV-88)

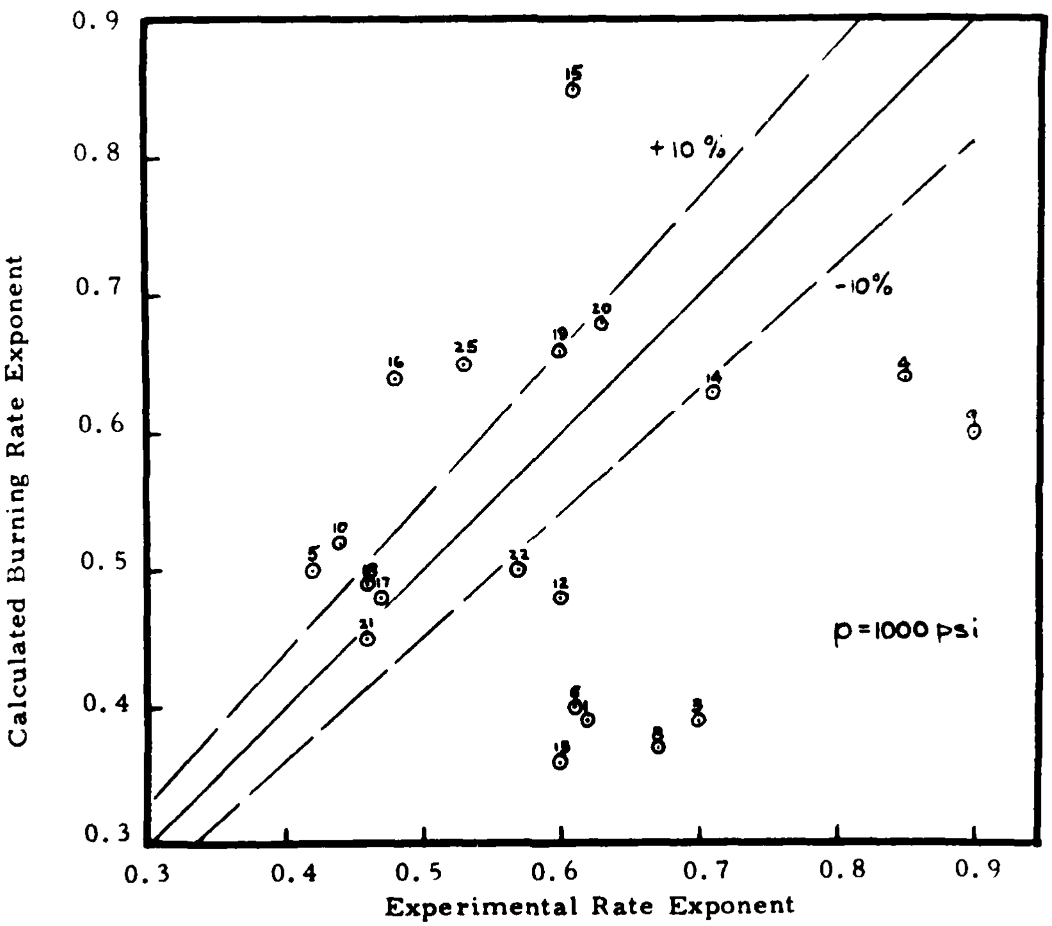

Figure 12. Burning Rate Exponent: Calculated versus Experimental for Miller's 90 micron Aluminum Additive Data Base (SD-IV-88)

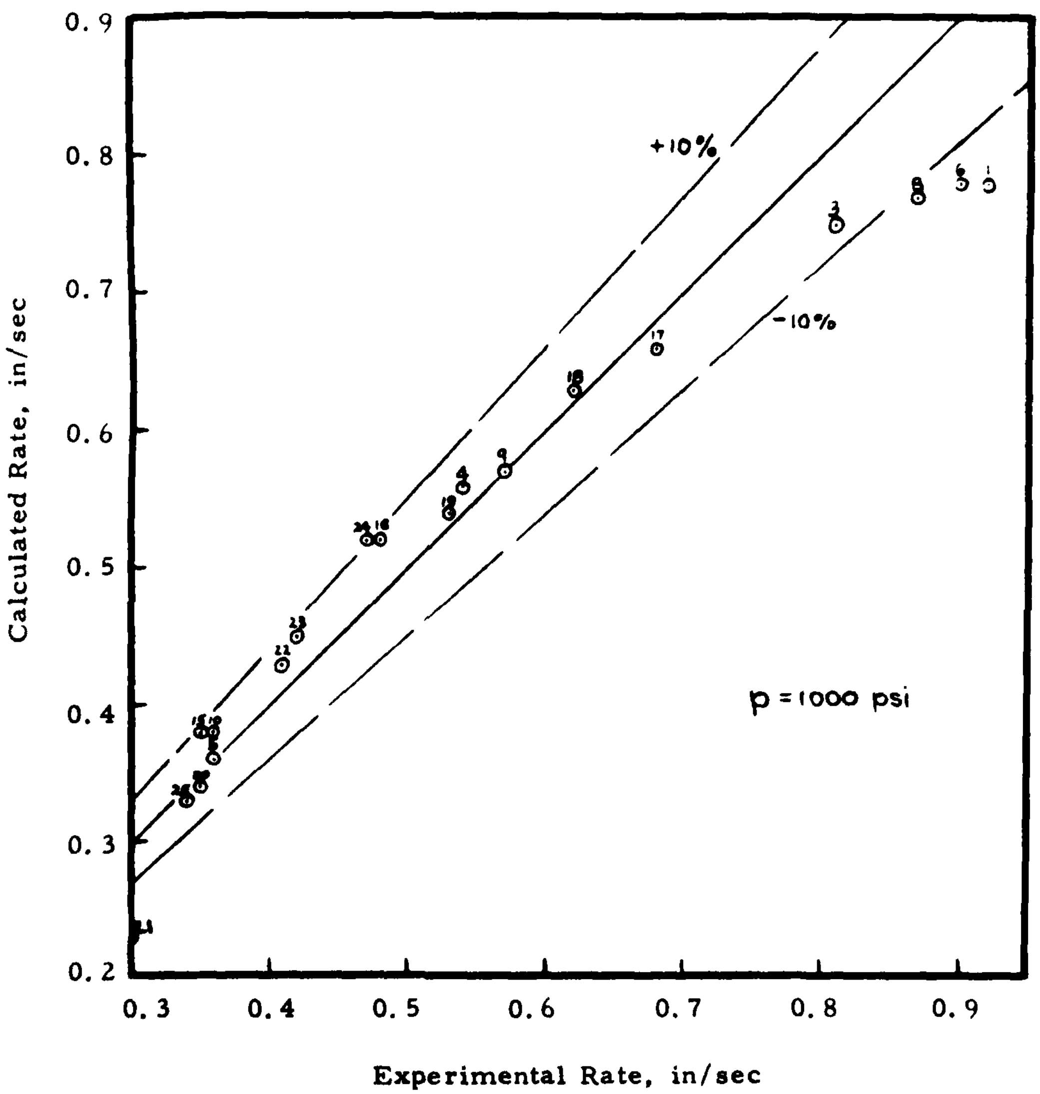

Figure 13. **Burning Rate: Calculated Versus Experimental for Miller's 6μ Aluminum Data Base (SD-V-88)**

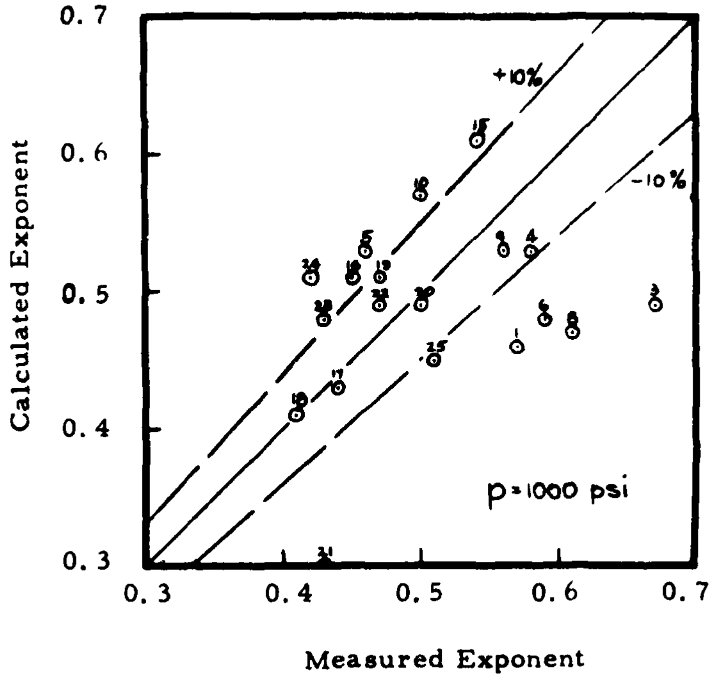

Figure 14. Exponent· Calculated Versus Experimental for Miller's 6μ Aluminum Data Base (SD-V-88)

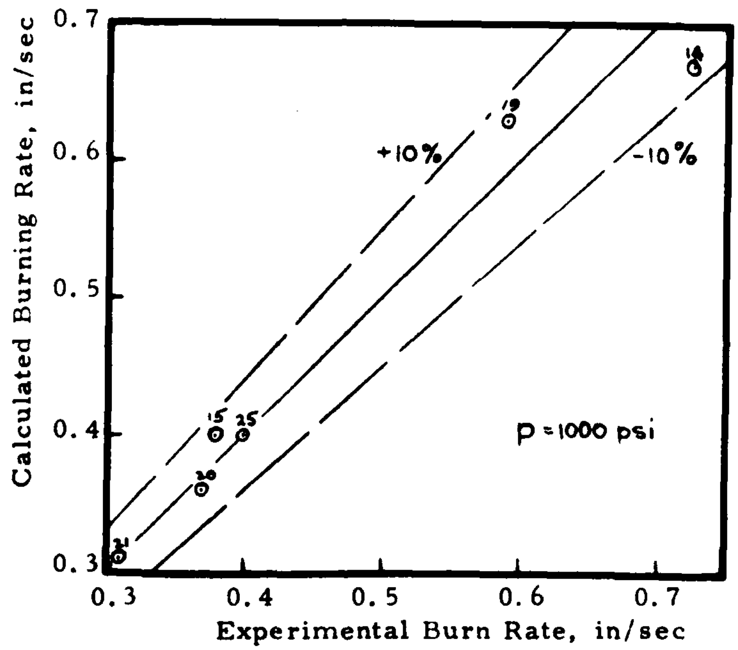

Figure 15. Burning Rate: Calculated versus Experimental for Miller's Extended Solids Data Base (SD-VI-90)

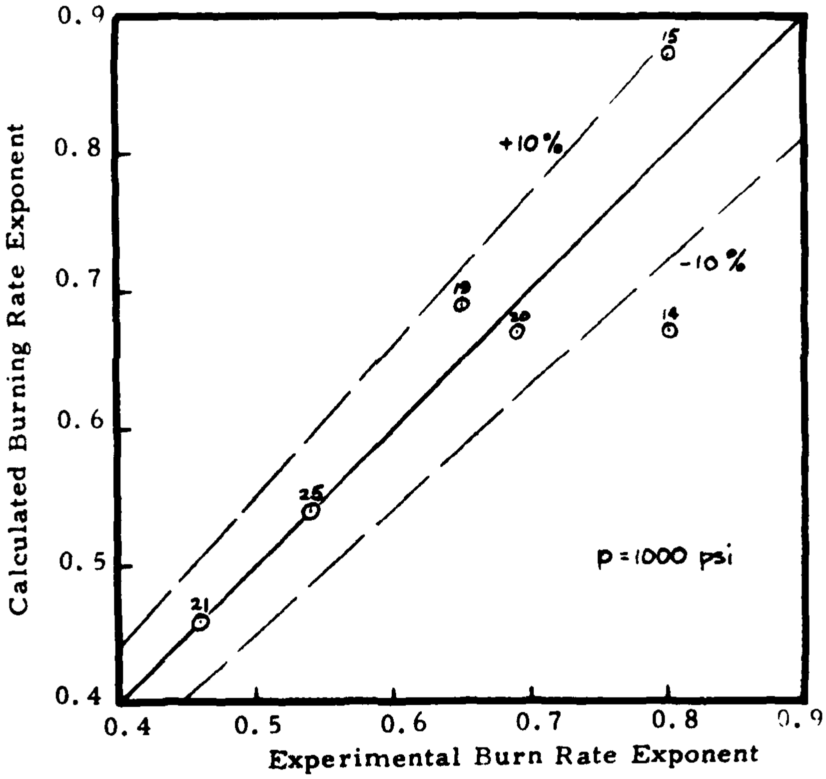

Figure 16. Burning Rate Exponent: Calculated versus Experimental for Miller's Extended Solids Data Base (SD-VI-90)

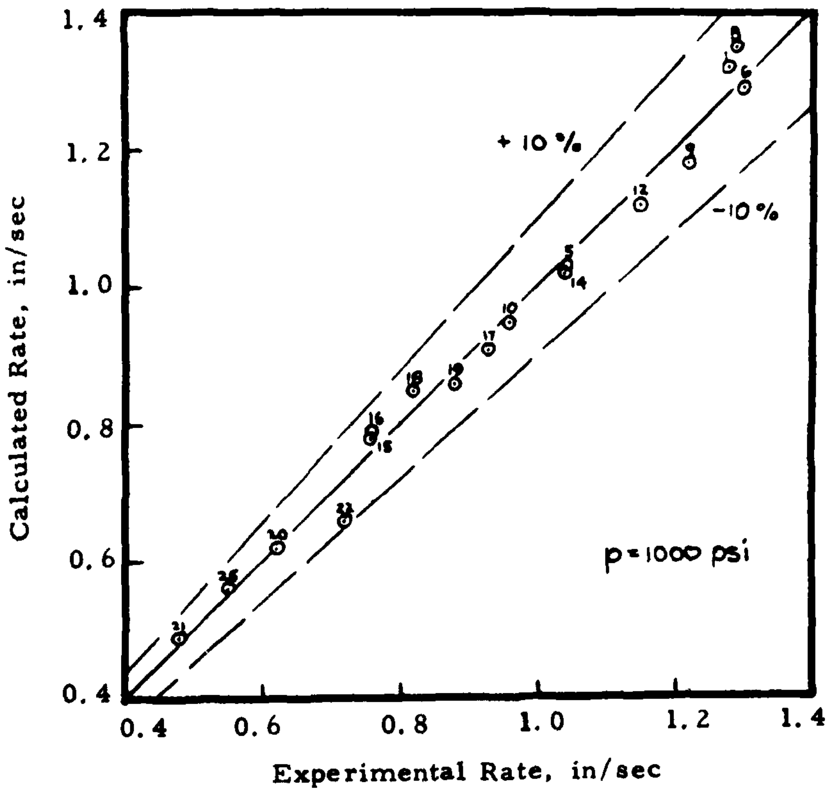

Figure 17. Burning Rate: Calculated Versus Experimental for Miller's 24μ Aluminum/Iron Oxide Data Base (SD-VII-88)

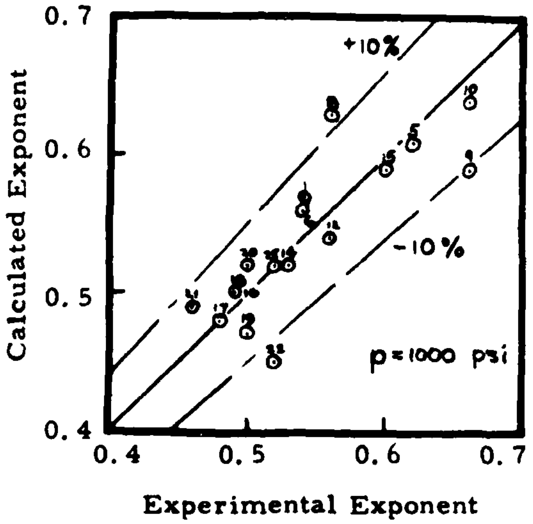

Figure 18. Exponent: Calculated Versus Experimental for Miller's 24μ Aluminum/Iron Oxide Data Base (SD VII-88)

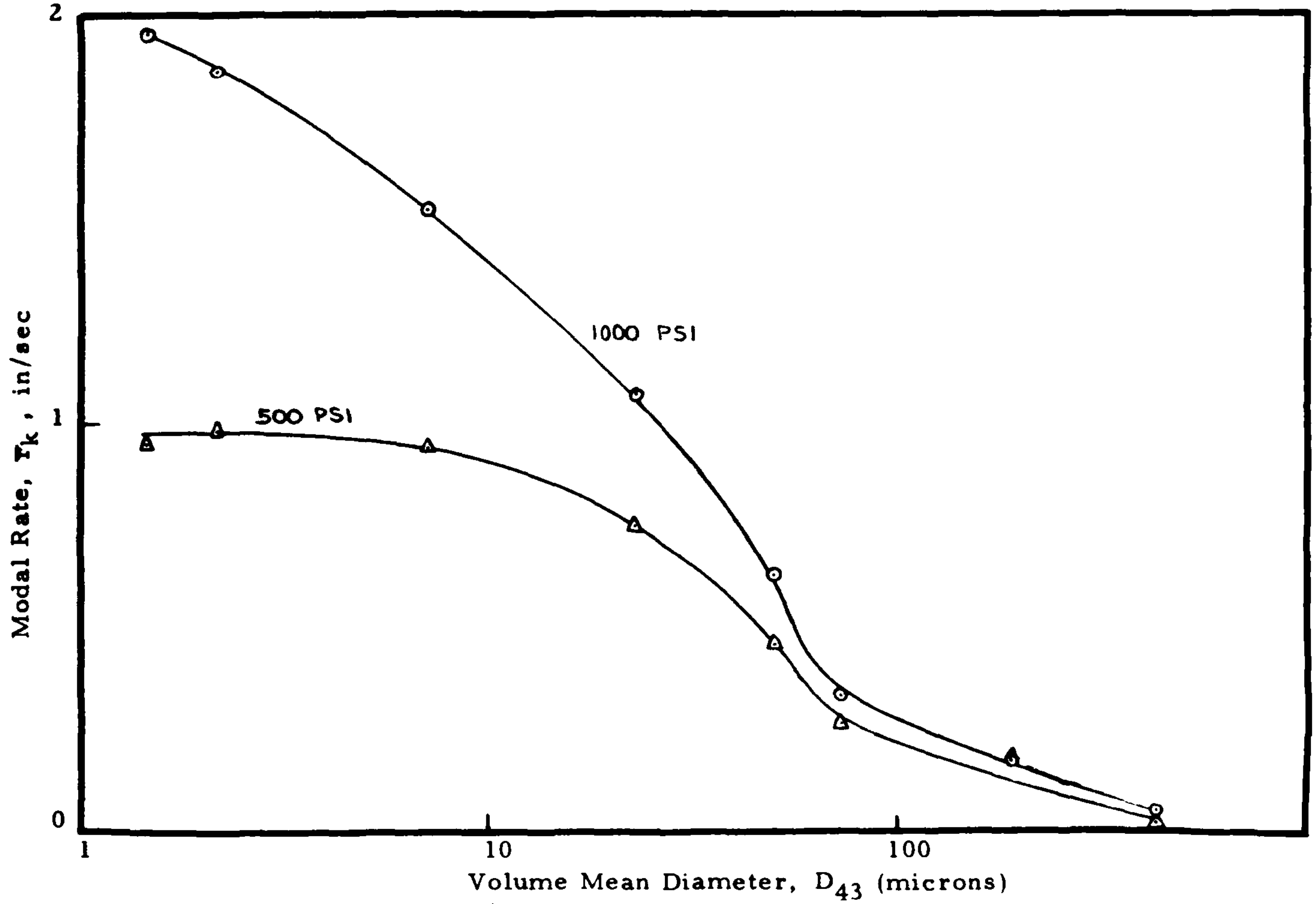

Figure 19. Variation of Modal Rates with Modal D_{43} (microns) for Miller's Additive Free Data Base (SD-III-88)

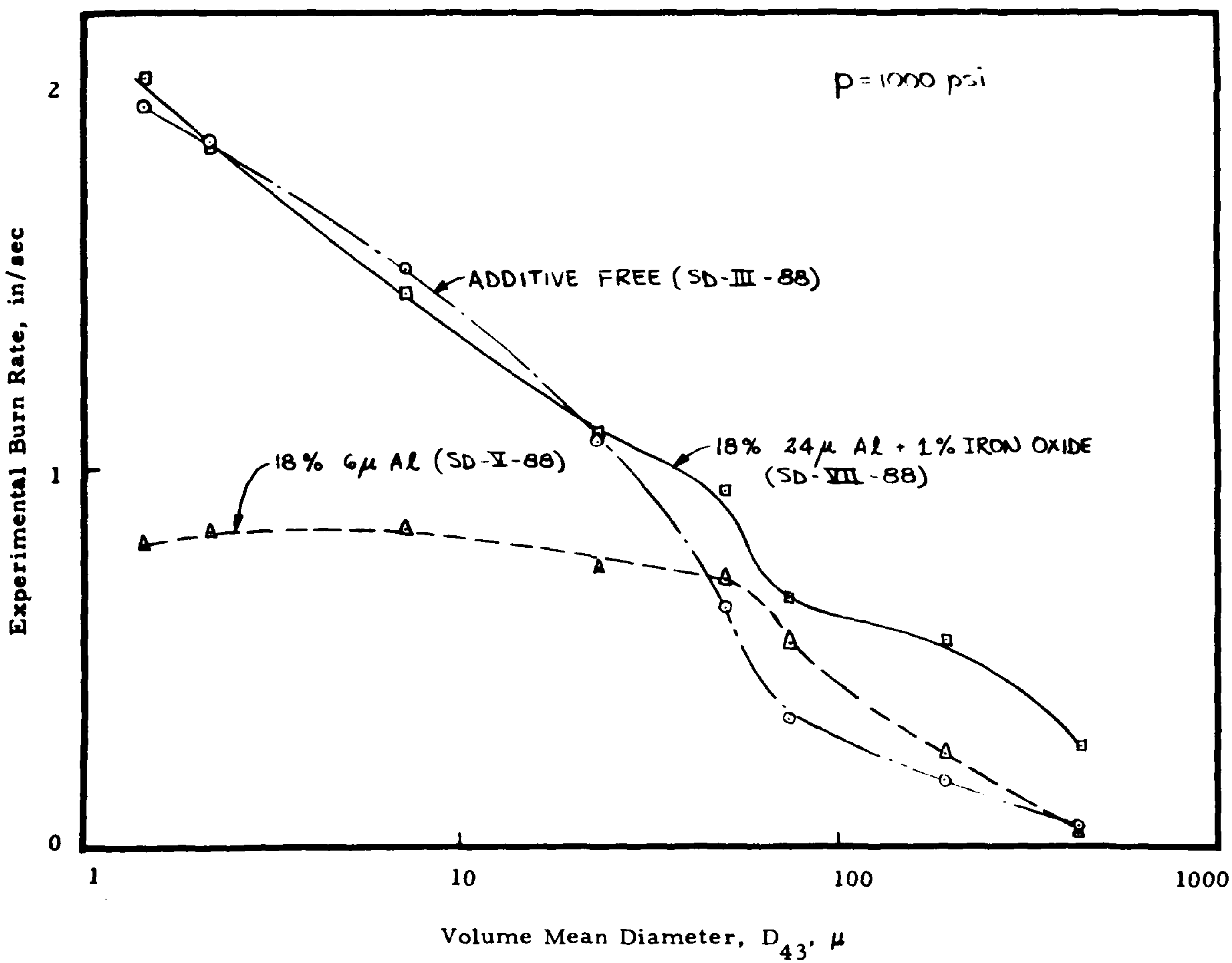

Figure 20. *Effect of Volume Mean Diameter on Burn Rate, Miller's Data Base*

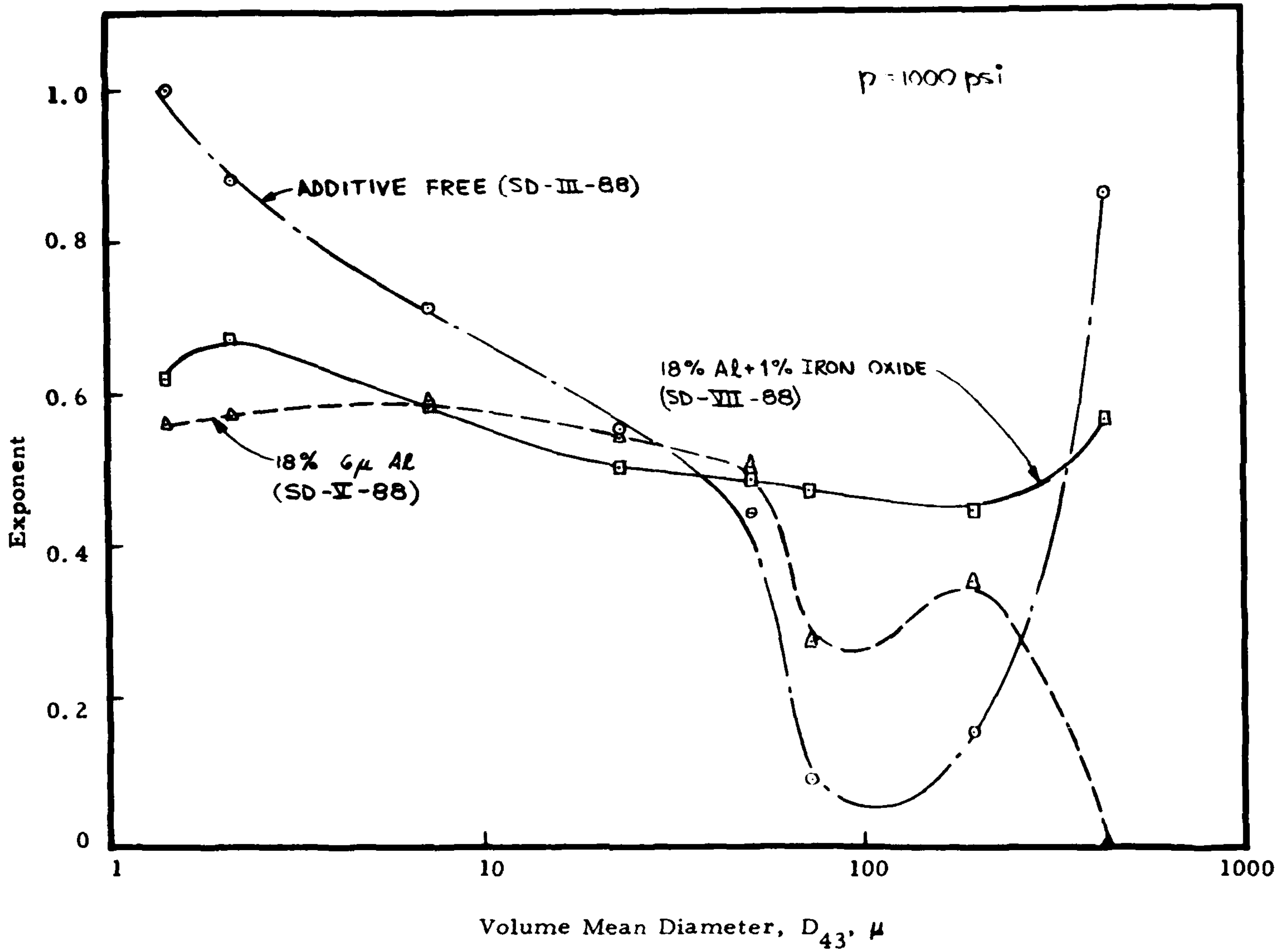

Figure 21. Effect of Volume Mean Diameter on Exponent, Miller's Data Base

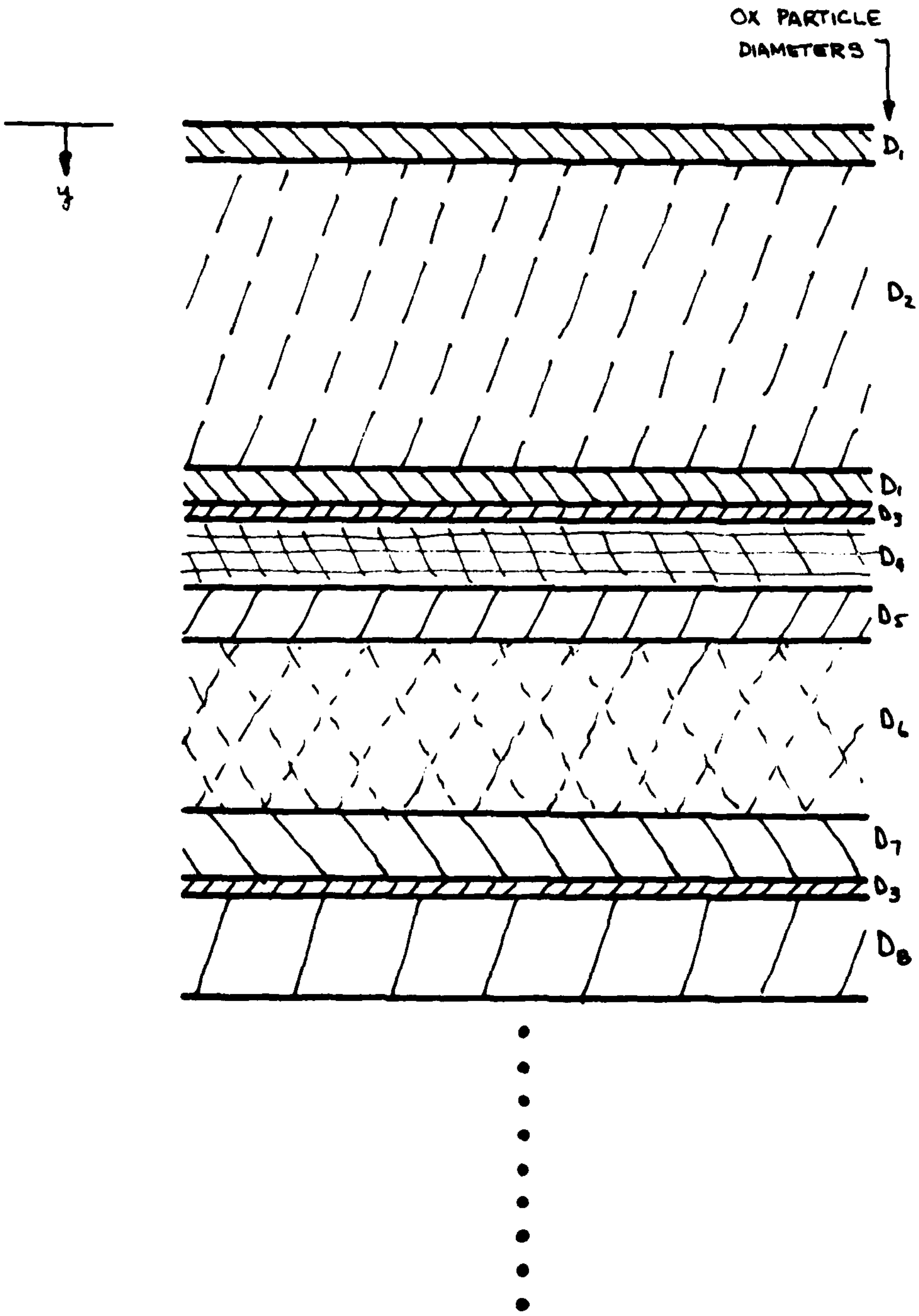

Figure 22. Schematic Illustrating Arrangement of Pseudopropellants

TABLE I

MODAL PROPERTIES FOR MILLER'S DATA BASE (1000 psi)

Formulation Designation	r_{400}	r_{200}	Modal Rates, in/sec* r_{90}	r_{50}	r_{20}	r_{6}	r_{2}	$r_{.7}$	Rate SEE**	n_{400}	n_{200}	Modal Exponents* n_{90}	n_{50}	n_{20}	n_{6}	n_{2}	$n_{.7}$	Exponent SEE**	Comments
SD-III-88	.053	.190	.336	.628	1.074	1.517	1.859	1.949	.050	.859	.156	.088	.435	.553	.706	.878	.995	.062	Additive Free
SD-I-88	0.000	.215	.524	.748	.737	.823	.714	.750	.147	.492	.652	.377	.475	.612	.642	.485	.529	.237	18% 24μ Al
SD-IV-88	.000	.319	.643	.693	.648	.751	.661	.709	.203	.623	.650	.322	.506	.631	.657	.493	.495	.271	18% 90μ Al
SD-V-88	.044	.257	.541	.714	.744	.840	.826	.792	.090	.001	.353	.272	.492	.537	.590	.571	.555	.157	18% 6μ Al
SD-VII-88	.273	.546	.662	.943	1.090	1.459	1.852	2.032	.034	.563	.447	.473	.483	.498	.576	.670	.620	.058	18% 24μ Al 1% Iron Oxide
SD-VI-90	.029	.404	--	.900	.794	.890	--	--	.048	.000	.423	--	.563	.731	.868	--	--	.080	21% 24μ Al

*Subscripts denote nominal diameter of mode in microns.
**Standard Error of Estimate

TABLE II

MODAL PROPERTIES FOR MAYKUT'S DATA BASE (1000 psi)

		Modal Rates, in/sec*				Modal Exponents*			
P psia	% Iron Oxide	r_{200}	r_{16}	$r_{1.7}$	Rate SEE**	n_{200}	n_{16}	$n_{1.7}$	Exponent SEE
700	0.5	0.000	0.907	1.273	.125				
700	0.75	0.021	0.839	1.665	.080				
700	2.0	0.137	1.050	1.611	.026				
1000	0.5	0.000	1.109	1.531	0.156	0.826	0.586	0.404	0.159
1000	0.75	0.000	.936	2.211	0.137	0.365	0.546	0.417	0.147
1000	2.0	0.179	1.215	2.158	0.020	0.331	0.433	0.593	0.018
2000	0.5	0.000	1.548	2.340	0.295				
2000	0.75	0.000	1.355	2.183	0.184				
2000	2.0	0.156	1.671	3.057	0.087				

*Subscripts denote nominal diameter of mode in microns.
**Standard Error of Estimate

APPENDIX A

NOMENCLATURE

D	particle diameter
E	error
$F_{ox,k}$	distribution function for the kth oxidizer mode
m	mass flux
M	number of oxidizer modes
n	pressure exponent
N	number of formulations
p	pressure
$q_{\bar{s}}$	heat flux at the burning surface in the condensed phase
r	burning rate
R_p	pressure coupled response function
t	time
T	temperature
y	spatial coordinate
α	oxidizer mass fraction
σ_p	temperature sensitivity at constant pressure

Subscripts

D	denotes particles with $D \leq D < D + \Delta D$
j	denotes jth formulation
k	denotes kth oxidizer mode
n	denotes exponent
o	denotes initial conditions
ox	denotes oxidizer
r	denotes rate
s	denotes conditions at burning surface
t	denotes total propellant

Special

$(\bar{\ })$	bar over denotes a mean value

APPENDIX B
MODAL PROPERTIES CODE

This computer program extracts modal properties from multi-modal propellant ballistic data according to the equations

$$\bar{r}_t = \sum_{k=1}^{M} \alpha_k \bar{r}_k / \alpha_t \qquad \text{B-1}$$

$$\bar{n}_t = \sum_{k=1}^{M} \alpha_k \bar{r}_k \bar{n}_k / (\alpha_t \bar{r}_t) \qquad \text{B-2}$$

where M is the number of oxidizer modes; α_k, $\bar{r}_k$, $\bar{n}_k$ are oxidizer mass fraction (mass ox/mass propellant), modal burn rate, and modal exponent respectively; α_t is the total oxidizer content; and $\bar{r}_t$ and $\bar{n}_t$ are the measured burning rate and pressure exponent respectively.

A nonlinear optimizer (PATSH) is employed to extract the "best" modal parameters $\bar{r}_k$, $\bar{n}_k$ $k = 1, M$ from a chemically consistent set of experimental data $\bar{r}_{t,j}$, $\alpha_{k,j}$, $\bar{n}_{t,j}$ $j = 1, N$ where $N \geq M$. A chemically consistent data set is one where all N formulations have the same chemical composition (variables are modal recipe and environment). The "best" $\bar{r}_k$, $\bar{n}_k$ is that which produces the smallest

$$E_r = \sqrt{\sum_{j=1}^{N} \left(\frac{\bar{r}_t - \bar{r}_{t,j}}{\bar{r}_{t,j}} \right)^2 / N}$$

for the $\bar{r}_k$ and the smallest

$$E_n = \sqrt{\sum_{j=1}^{N} \left(\frac{\bar{n}_t - \bar{n}_{t,j}}{\bar{n}_{t,j}} \right)^2 / N}$$

for the $\bar{n}_k$.

Here $\bar{r}_{t,j}$, $\bar{n}_{t,j}$ refers to test data and $\bar{r}_t$, $\bar{n}_t$ to calculated (by Eqs. B.1 and B.2) results for the jth formulation. The "search" for the $\bar{r}_k$ begins with $\bar{r}_k = \bar{r}_{k+1} = \bar{r}_{t,1}$ and $\bar{n}_k = \bar{n}_{k+1} = \bar{n}_{t,1}$.

The input format consists of two major units. The first card defines the number of oxidizer modes, the number of formulations with these modes, the number of pressures at which data was obtained, and those pressures. Subsequent cards tabulate recipe, rate, and exponent for each formulation and pressure in the sequence. Figure B.1 illustrates a typical data set.

Output consists of the standard error of estimate of the fits and the r_k, n_k $k = 1, M$. Figure B. 2 illustrates results obtained from the Figure B. 1 data set. Figure B. 3 lists the Fortran IV code.

```
  MILLER DATA SET SD-III-1,-25 (ZERO ADDITIVE)
0821031000.500. 2000.
          .3158       .1368              .4211 .9161.165 .6271.214          -02
                      .5579              .3158 .6891.446 .3312.291          -03
     .3158            .2421              .3158 .7971.168 .6321.909          -04
.4211                 .1368              .3158 .928  .870 .4711.704         -05
               .3158.1368.3158.1053            .6211.160 .7371.744          -06
               .3158.2421     .3158            .6921.096 .6801.774          -08
     .3158            .2421   .3158            .7711.087 .6311.822          -09
.4211                 .1368   .3158            .841  .901 .5001.604         -10
          .3158       .1368.4211               .6171.030 .6761.589          -12
     .3158            .2421.3158               .613  .978 .6371.490         -14
.4211                 .1368.3158               .690  .706 .4491.169         -15
     .3158     .3158.2421                      .451  .561 .407 .761         -16
          .3158       .5579                    .474  .834 .6011.158         -17
          .4211       .4526                    .437  .718 .521  .955        -18
     .3158            .5579                    .529  .755 .5361.116         -19
.4211                 .4526                    .610  .539 .368 .856         -20
.3158.3158     .1053.1368                      .430  .330 .240 .436         -21
.3158          .4211.1368                      .458  .524 .375 .708         -22
     .4211     .3158.1368                      .463  .469 .332 .630         -23
     .3158     .4211.1368                      .449  .536 .393 .732         -24
.4211          .3158.1368                      .528  .445 .304 .652         -25
```

Figure B.1 - Input Format for Code

MILLER DATA SET SD-III-1.-25 (ZERO ADDITIVE)

CX MASS FRACTION DATA ** EXPERIMENT, RATE DATA

MODE 1	MODE 2	MODE 3	MODE 4	MODE 5	MODE 6	MODE 7	MODE 8	K(P1)	F(P1)	F(P2)	F(P3)	F(P4)	F(P5)
0.0	0.0	0.3158	0.0	0.1368	0.0	0.0	0.4211	[illegible]	[illegible]	[illegible]	[illegible]		
0.0	0.0	0.0	0.0	0.5579	0.0	0.0	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]		
0.0	0.3158	0.0	0.0	0.2421	0.0	0.0	[illegible]	[illegible]	[illegible]	[illegible]	[illegible]		
0.4211	0.0	0.0	0.0	0.1368	0.0	0.0	0.3158	[illegible]	[illegible]	0.4710	1.7040		
0.0	0.0	0.0	0.3158	0.1368	0.3158	0.1053	0.0	0.7210	1.1600	0.7370	1.7440		
0.0	0.0	0.0	0.3158	0.2421	0.0	0.3158	0.0	0.6920	[illegible]	0.6800	1.7740		
0.0	0.3158	0.0	0.0	0.2421	0.0	0.3158	0.0	0.7710	1.0470	0.7210	[illegible]		
0.4211	0.0	0.0	0.0	0.1368	0.0	0.3158	0.0	0.6410	[illegible]	0.5000	1.6040		
0.0	0.0	0.3158	0.0	0.1368	0.4211	0.0	0.0	0.6170	[illegible]	0.6740	1.5800		
0.0	0.3158	0.0	0.0	0.2421	0.3158	0.0	0.0	0.6130	0.9780	0.6370	1.4900		
0.4211	0.0	0.0	0.0	0.1368	0.3158	0.0	0.0	0.6900	0.7060	0.6490	1.1690		
0.0	0.3158	0.0	0.3158	0.2421	0.0	0.0	0.0	0.4510	0.5610	0.4070	0.7610		
0.0	0.0	0.3158	0.0	0.5579	0.0	0.0	0.0	0.4740	0.4340	[illegible]	1.1590		
0.0	0.0	0.4211	0.0	0.4526	0.0	0.0	0.0	0.4370	0.7130	0.5210	0.9550		
0.0	0.3158	0.0	0.0	0.5579	0.0	0.0	0.0	0.5290	0.7850	0.5350	1.1160		
0.4211	0.0	0.0	0.0	0.4526	0.0	0.0	0.0	0.6100	0.5390	0.3680	0.8560		
0.3158	0.3158	0.0	0.1053	0.1368	0.0	0.0	0.0	0.4300	0.3300	0.2400	0.4360		
0.3158	0.0	0.0	0.4211	0.1368	0.0	0.0	0.0	0.4580	0.5240	0.3750	0.7080		
0.0	0.4211	0.0	0.3158	0.1368	0.0	0.0	0.0	0.4430	0.4690	0.3320	0.6300		
0.0	0.3158	0.0	0.4211	0.1368	0.0	0.0	0.0	0.4490	0.5360	0.3930	0.7320		
0.4211	0.0	0.0	0.3158	0.1368	0.0	0.0	0.0	0.5230	0.4450	0.3040	0.6520		

Figure B. 2 - Sample Output

MILLER DATA SET SD-III-1.-25 (ZERO ADDITIVE)

P =1000.0 PSI   RATE STD ERR= 4.9882E-02   EXPONENT STD ERR= 6.1590E-02

*   COMPUTED MODAL RATES, IN/SEC   **   COMPUTED MODAL EXPONENTS   *

RM1	RM2	RM3	RM4	RM5	RM6	RM7	RM8	NM1	NM2	NM3	NM4	NM5	NM6	NM7	NM8
-0.0525	0.1896	0.3358	0.6277	1.0735	1.5172	1.8594	1.9486	0.8593	0.1526	-0.0884	0.4352	0.5526	0.7056	0.8783	0.9950

*   COMPARISON THEORY/EXPERIMENT   *

R	RC	ERR	N	NC	ERN
1.1650	1.2268	-0.0530	0.9160	0.8879	0.0307
1.4460	1.3884	0.0398	0.6890	0.7447	-0.0808
1.1680	1.0690	0.0848	0.7970	0.7473	0.0623
0.8700	0.8963	-0.0303	0.9280	0.9341	-0.0066
1.1600	1.1674	-0.0064	0.6210	0.6695	-0.0764
1.0960	1.1964	-0.0916	0.6920	0.7787	-0.1252
1.0870	1.0381	0.0450	0.7710	0.7039	0.0870
0.9010	0.8654	0.0355	0.8410	0.7824	0.0657
1.0300	1.0207	0.0090	0.6170	0.6016	0.0250
0.9780	0.9144	0.0650	0.6130	0.5744	0.0629
0.7060	0.7418	-0.0507	0.6900	0.7105	-0.0297
0.5610	0.5929	-0.0568	0.4510	0.4876	-0.0812
0.8340	0.8069	0.0325	0.4740	0.4671	0.0146
0.7180	0.7180	0.0001	0.4370	0.4479	-0.0250
0.7850	0.7540	0.0395	0.5290	0.4959	0.0626
0.5390	0.5814	-0.0787	0.6100	0.6105	-0.0008
0.3300	0.3312	-0.0038	0.4300	0.4623	-0.0751
0.5240	0.4896	0.0657	0.4580	0.4596	-0.0035
0.4690	0.4864	-0.0370	0.4630	0.4383	0.0534
0.5360	0.5391	-0.0059	0.4490	0.4384	0.0236
0.4450	0.4203	0.0556	0.5280	0.4794	0.0920

Figure B.2 - Sample Output (continued)

```
MILLER DATA SET SD-III-1.-25 (ZERO ADDITIVE)

P = 500.0 PSI     RATE STD ERR= 4.7113E-02     EXPONENT STD ERR= 6.1590E-02

*              COMPUTED MODAL RATES, IN/SEC                **                 COMPUTED MODAL EXPONENTS                *

  RM1      RM2      RM3      RM4      RM5      RM6      RM7      RM8      NM1      NM2      NM3      NM4      NM5      NM6      NM7      NM8

-0.0276   0.1434   0.2674   0.4581   0.749C   0.9413   0.9800   C.9468

*          COMPARISON THEORY/EXPERIMENT          *

   R        RC       ERR        N         NC        ERR

C.6270   0.6705  -0.0694
0.8810   0.8207   0.C685
0.6320   0.6018   0.0478
C.4710   C.4730  -0.0042
0.7370   0.7412  -0.0057
0.6800   0.7274  -0.0696
0.6310   0.6136   0.C276
0.5000   0.4848   0.0304
0.6760   0.6676   0.0124
0.6370   0.5996   0.0587
0.4490   0.4708  -0.0486
0.4070   0.4249  -0.0441
0.6010   0.5749   0.0434
0.5210   0.5169   0.0079
0.5360   0.5301   0.C11C
0.3680   0.4013  -0.0904
0.2400   0.2343   0.C239
0.3750   0.3480   0.0719
0.3320   0.3520  -0.0601
0.3930   0.3899   0.C079
0.3040   0.2961   0.0258
```

Figure B.2- Sample Output (continued)

MILLER DATA SET SD-III-1.-25 (ZERO ADDITIVE)

P =2000.0 PSI   RATE STD ERR= 4.4083E-02   EXPONENT STD ERR= 5.1590E-02

*   COMPUTED MODAL RATES, IN/SEC   **   COMPUTED MODAL EXPONENTS   *

RM1	RM2	RM3	RM4	RM5	RM6	RM7	RM8	NM1	NM2	NM3	NM4	NM5	NM6	NM7	NM8
-0.1396	-0.1732	0.3480	0.8300	1.5668	2.4713	3.3515	3.8095								

*   COMPARISON THEORY/EXPERIMENT   *

R	RC	ERR	N	NC	ERN
2.2140	2.2071	0.0031			
2.2910	2.3773	-0.0377			
1.9090	1.8735	0.0185			
1.7040	1.6895	0.0085			
1.7440	1.8425	-0.0565			
1.7740	1.9456	-0.0967			
1.8220	1.7082	0.0625			
1.6040	1.5240	0.0499			
1.5890	1.5622	0.0169			
1.4900	1.3900	0.0671			
1.1690	1.2059	-0.0315			
0.7610	0.7968	-0.0470			
1.1580	1.1263	0.0274			
0.9550	0.9794	-0.0255			
1.1160	1.0631	0.0474			
0.8560	0.8790	-0.0268			
0.4360	0.4584	-0.0515			
0.7080	0.6958	0.0172			
0.6300	0.6288	0.0019			
0.7320	0.7080	0.0328			
0.6520	0.6126	0.0604			

Figure B.2 - Sample Output (concluded)

```
0001          EXTERNAL MODER1,MODEN1
0002          DIMENSION NM(8),HEAD(20),P(5),RMK(8)
0003          COMMON/MADER/ II,JJ,ALFA(8,50),R(50,5),N(50),RC(50),ALFAT(50),
             1         RM(8,5),NC(50),K,ERR(50),ERN(50)
0004          REAL N,NM,NC
        C R(J,K)    EXPERIMENTAL BURN RATES FOR THE JTH FORMULATION AND P(K)
        C N(J)      EXPERIMENTAL PRESSURE EXPONENT FOR THE JTH FORMULATION AND
        C           P(I)
        C RC(J)     CALCULATED BURN RATE FOR THE JTH FORMULATION AND P(K)
        C NC(J)     CALCULATED EXPONENT FOR THE JTH FORMULATION AND P(K)
        C ERR1      STANDARD DEVIATION OF RC FROM R FOR P(K)
        C ERR2      STANDARD DEVIATION OF NC FROM N FOR P(K)
        C RM(I,K)   MODAL BURNING RATE FOR ITH MODE  AND P(K)
        C NM(I)     PRESSURE EXPONENT FOR THE ITH MODE AND P(I)
        C ALFA(I,J) MASS FRACTION OF ITH MODE OXIDIZER IN JTH FORMULATION
        C ALFAT(J)  TOTAL OXIDIZER CONTENT OF JTH FORMULATION
        C II        NUMBER OF OX MODES < 8
        C JJ        NUMBER OF FORMULATIONS < 50
        C KK        NUMBER PRESSURES RATE DATA AVAILABLE < 5
        C ERR(J)    ERROR BETWEEN R(J,K) AND RC(J) AT P(K)
        C ERN(J)    ERROR BETWEEN N(J) AND NC(J) FOR P(I)
        C
        C THEORY ASSUMES THAT
        C      R(J)=SUM(ALFA(I,J)*RM(I))/SUM(ALFA(I,J))
        C      N(J)=SUM(ALFA(I,J)*RM(I)*NM(I))/SUM(ALFA(I,J)*RM(I))
        C
        C ROBERT LAIN GLICK    AUGUST 3, 1977
        C
        C INPUT JOB HEADING AND PRINT OUT THAT HEADING
        C
0005        1 READ(5,10,END=210) HEAD
0006       10 FORMAT(20A4)
0007          WRITE(6,11) HEAD
0008       11 FORMAT(1H1,20A4,//2H *20X,'OX MASS FRACTION DATA',21X,2H**,21X
             1,'EXPONENT,RATE DATA',23X,1H*,//3X,'MODE 1',2X,'MODE 2',2X,'MODE 3'
             2,2X,'MODE 4',2X,'MODE 5',2X,'MODE 6',2X,'MODE 7',2X,'MODE 8',3X,
             3'N(P1)',3X,'R(P1)',3X,'R(P2)',3X,'R(P3)',3X,'R(P4)',3X,'R(P5)',/)
        C
        C INPUT DATA
        C
0009          READ(5,20) II,JJ,KK,(P(K),K=1,KK)
0010       20 FORMAT(3I2,5F5.4)
0011          DO 60 J=1,JJ
0012          READ(5,30) (ALFA(I,J),I=1,8),N(J),(R(J,K),K=1,KK)
0013       30 FORMAT(14F5.4)
        C
        C OUTPUT INPUT DATA
        C
0014          WRITE(6,40) (ALFA(I,J),I=1,II)
0015       40 FORMAT(1H ,8F8.4)
0016          WRITE(6,50) N(J),(R(J,K),K=1,KK)
0017       50 FORMAT(1H+,64X,6F8.4)
0018       60 CONTINUE
        C
        C RESET KPRINT FOR NM(I) DETERMINATION
        C
0019          KPRINT=1
        C
```

Figure B.3 - Computer Code

```
              C COMPUTE ALFAT(J)
              C
0020                DO 67 J=1,JJ
0021                ALFAT(J)=0.0
0022                   DO 63 I=1,II
0023                   ALFAT(J)=ALFAT(J)+ALFA(I,J)
0024             63    CONTINUE
0025             67 CONTINUE
              C
              C FIND RM(I,K) FOR EACH P(K)
              C
0026                DO 200 K=1,KK
              C
              C SET INITIAL RM(I,K)
              C
0027                   DO 70 I=1,II
0028                   RMA(I)=R(I,K)
0029                   IF(K .EQ. 1) NM(I)=N(I)
0030             70    CONTINUE
              C
              C FIND OPTIMAL RM(I,K)
              C
0031             80 CALL PATSH(RMA,ERR1,II,5.0,0.001,50,-1,MODER1)
0032                   DO 90 I=1,II
0033             90    RM(I,K)=RMA(I)
              C
              C NEED FIND NM(I) ?
              C
0034                IF(K .GT. 1) KPRINT=2
0035                IF(N(1) .EQ. 0.0) KPRINT=2
0036                IF(KPRINT .EQ. 2) GO TO 100
              C
              C FIND OPTIMAL N(I)
              C
0037                CALL PATSH(NM,ERR2,II,5.0,0.001,50,-1,MODEN1)
              C
              C OUTPUT COMPUTED RESULTS THIS P(K)
              C
0038            100 WRITE(6,110) HEAD
0039            110 FORMAT(1H1,20A4)
0040                WRITE(6,115) P(K),ERR1,ERR2
0041            115 FORMAT(1H0,3HP =,F6.1,4H PSI,5X,'RATE STD ERR=',1PE11.4,5X,'EXPONE
                   1NT STD ERR=',1PE11.4///2H *,16X,'COMPUTED MODAL RATES, IN/SEC',18X,
                   22H**,18X,'COMPUTED MODAL EXPONENTS',21X,1H*,//4X,'RM1',5X,'RM2',5X
                   3,'RM3',5X,'RM4',5X,'RM5',5X,'RM6',5X,'RM7',5X,'RM8',5X,'NM1',5X,
                   4'NM2',5X,'NM3',5X,'NM4',5X,'NM5',5X,'NM6',5X,'NM7',5X,'NM8',//)
0042                WRITE(6,120) (RM(I,K),I=1,II)
0043            120 FORMAT(1H , 8F8.4)
0044                IF(KPRINT .EQ. 1) WRITE(6,130) (NM(I),I=1,II)
0045            130 FORMAT(1H+,64X, 8F8.4)
0046                WRITE(6,140)
0047            140 FORMAT(2H0*,10X,'COMPARISON THEORY/EXPERIMENT',9X,1H*//5X,'R',7X,
                   1'RC',5X,'ERR',6X,'N',7X,'NC',5X,'ERN',/)
0048                   DO 180 J=1,JJ
0049                   WRITE(6,150) R(J,K),RC(J),ERR(J)
0050            150    FORMAT(1H  3F8.4)
0051                   IF(KPRINT .EQ. 1) WRITE(6,160) N(J),NC(J),ERN(J)
0052            160    FORMAT(1H+ ,24X,3F8.4)
```

Figure B.3 - Computer Code (continued)

```
FORTRAN IV G LEVEL  21                MAIN              DATE = 77258          14/39/43           PAGE 0003

0053           180    CONTINUE                                                       00001170
0054              KPRINT=1                                                           00001180
0055           200 CONTINUE                                                          00001190
0056               GO TO 1                                                           00001200
0057           210 STOP                                                              00001210
0058               END                                                               00001220
```

Figure B.3 - Computer Code (continued)

```
FORTRAN IV G LEVEL  21                MODER1            DATE = 77258          14/39/43                PAGE 0001

0001           SUBROUTINE MODER1(RMA,ERR1)
0002           COMMON/MADER/II,JJ,ALFA(8,50),R(50,5),N(50),RC(50),ALFAT(50)
              1        ,RM(8,5),NC(50),K,ERR(50),ERN(50)
0003           DIMENSION RMA(8)
         C THIS SUBROUTINE COMPUTES STANDARD DEVIATION BETWEEN R(J,K) AND RC(J)
         C FOR P(K)
         C WHERE
         C  R(J,K)       EXPERIMENTAL BURNING RATE FOR JTH FORMULATION AT P(K)
         C  RC(J)        THEORETICAL BURNING RATE FOR JTH FORMULATION AT P(K)
         C  RMA(I)       BURNING RATE FOR ITH MODE OF FORMULATION AT P(K)
         C  ALFA(I,J)    MASS FRACTION OF ITH MODE OX IN JTH FORMULATION
         C  ALFAT(J)     TOTAL OX MASS FRACTION IN JTH FORMULATION
         C  II           NUMBER OF OX MODES < 8
         C  JJ           NUMBER OF FORMULATIONS < 50
         C  ERR(J)       ERROR BETWEEN R(J,K) AND RC(J) AT P(K)
         C  ERR1         STANDARD ERROR OF ESTIMATE FOR DATA SET R AND RC
         C
         C ROBERT LAIN GLICK  AUGUST 3, 1977
         C
         C
0004        10 ERR1=0.00
0005        15 DO 30 J=1,JJ
               RC(J)=0.0
0006        20   DO 25 I=1,II
0007        25   RC(J)=RC(J)+ALFA(I,J)*ABS(RMA(I))
0008             RC(J)=RC(J)/ALFAT(J)
0009     C COMPUTE ABSOLUTE ERROR
         C     ERR(J)=R(J,K)-RC(J)
         C COMPUTE RELATIVE ERROR
0010           ERR(J)=(R(J,K)-RC(J))/R(J,K)
0011           ERR1=ERR1+ERR(J)*ERR(J)
0012        30 CONTINUE
0013           ERR1=SQRT(ERR1/JJ)
0014           RETURN
0015           END
```

Figure B.3 - Computer Code (continued)

```
FORTRAN IV G LEVEL  21                MODEN1            DATE = 77258         14/39/43              PAGE 0001

0001            SUBROUTINE MODEN1(NM,ERR2)
0002            DIMENSION NM(8)
0003            COMMON/MADER/II,JJ,ALFA(8,50),R(50,5),N(50),RC(50),ALFAT(50)
               1         ,RM(8,5),NC(50),K,ERR(50),ERN(50)
0004            REAL N,NM,NC
          C
          C THIS SUBROUTINE FINDS THE STANDARD DEVIATION BETWEEN N(J) AND NC(J)
          C
          C   N(J)        EXPERIMENTAL EXPONENT FOR JTH FORMULATION AT P(1)
          C   NC(J)       THEORETICAL EXPONENT FOR JTH FORMULATION
          C   RM(I,K)     BURNING RATE FOR THE ITH MODE AT P(K)
          C   NM(I)       EXPONENT FOR THE ITH MODE AT P(1)
          C   ALFA(I,J)   MASS FRACTION OF ITH OX MODE IN JTH FORMULATION
          C   ALFAT(J)    TOTAL MASS FRACTION OF OX IN JTH FORMULATION
          C   II          NUMBER OF MODES <8
          C   JJ          NUMBER OF FORMULATIONS < 50
          C   ERN(J)      ERROR BETWEEN N(J) AND NC(J)
          C   ERR2        STANDARD ERROR OF ESTIMATE FOR DATA SET N AND NC
          C
          C  ROBERT LAIN GLICK   AUGUST 3, 1977
          C
          C
0005          5 ERR2=0.0
0006         10 DO 30 J=1,JJ
0007            NC(J)=0.0
0008              DO 25 I=1,II
0009         25   NC(J)=NC(J)+ABS(RM(I,1)*NM(I))*ALFA(I,J)
          C CALCULATE EXPONENT USING MEASURED RATE
0010            NC(J)=NC(J)/ALFAT(J)/R(J,1)
          C CALCULATE EXPONENT USING CALCULATED RATE
          C     NC(J)=NC(J)/ALFAT(J)/RC(J)
          C CALCULATE ABSOLUTE ERROR
          C     ERN(J)=N(J)-NC(J)
          C CALCULATE RELATIVE ERROR
0011            ERN(J)=(N(J)-NC(J))/N(J)
0012         30 ERR2=ERR2 + ERN(J)*ERN(J)
0013            ERR2=SQRT(ERR2/JJ)
0014            RETURN
0015            END
```

Figure B.3 - Computer Code (continued)

```
FORTRAN IV G LEVEL  21                PATSH              DATE = 77258         14/39/43                PAGE 0001

0001             SUBROUTINE PATSH(PSI,SSI,N,DELS,DLMIN,ITLIM,IPT,WRIT4)
           C THIS VERSION OF PATSH HAS BEEN ALTERED FROM THE WOLTOSZ VERSION TO
           C CONFORM TO THE CALLING SEQUENCE OF THE ORIGINAL CODE (SEE MIT WRITEUP)
           C     COMMON/OPTIM/N,DELS,DLMIN,ITLIM,IPT
0002             DIMENSION PSI(25),PHI(25),THT(25),XFLG(25)
0003             DATA IPR/6/
0004             DATA ALFA/1.02/
0005             F(SSS)=SSS-ABS(SSS)*.0001*CUT
           C THE ITWICE PARAMETER ADDED BY WOLTOSZ HAS BEEN SPECIFIED HERE
0006             ITWICE=1
0007             DEL=DELS
0008             IF (IPT.GE.0) WRITE(IPR,604) DEL,DLMIN,ITLIM,IPT
0009             DO 705 I=1,N
0010         705 XFLG(I)=1.
0011             ITER=0
0012             CUT=1.
0013          10 CALL WRIT4(PSI,SSI)
0014        90   SSITST=F(SSI)
0015         100 S=SSI
0016             NPATH=0
0017             DO 101 I=1,N
0018         101 PHI(I)=PSI(I)
0019             ICALL=1
0020             IF (IPT.LT.0) GO TO 150
0021             WRITE(IPR,599) ITER
0022             WRITE(IPR,600) (PSI(J),J=1,N)
0023             WRITE(IPR,601)  S,DEL
0024             GO TO 150
0025        160  IF(S.LT.SSITST) GO TO 200
0026             DEL=DEL/2.
0027             IF(DEL.GT.DLMIN) GO TO 100
0028             IF(IPT.GE.0) WRITE(IPR,704)
0029             IF(CUT.LT..5) GO TO 702
0030             CALL WRIT4(PHI,SPI)
0031             IF(IPT.GE.0) WRITE(IPR,707)
0032             IF(ITWICE.EQ.0)RETURN
0033             DEL=DELS
0034             CUT=0.
0035             GOTO 90
0036         200 SSI=S
0037             SSITST=F(SSI)
0038             ITER=ITER+1
0039             NPATH=NPATH+1
0040             IF(ITER.GT.ITLIM) GO TO 700
0041             IF(IPT.LT.0) GO TO 203
0042             WRITE(IPR,599) ITER
0043             WRITE(IPR,599) NPATH
0044             WRITE (IPR,600) (PHI(I),I=1,N)
0045             WRITE (IPR,601) SSI,DEL
0046             IF(IBPPRT.LT.1)GO TO 203
0047             IAPSV=IAPRT
0048             IMPSV=IMPRT
0049             IF(IBPPRT.GT.1)IAPRT=1
0050             IMPRT=1
0051             CALL WRIT4(PSI,SPI)
0052             IMPRT=IMPSV
0053             IAPRT=IAPSV
           C MAKE PATTERN MOVE
```

Figure B.3 - Computer Code (continued)

```
0054        203   DO 201 I=1,N
0055              THT(I)=PSI(I)
0056              PSI(I)=PHI(I)
0057        201   PHI(I)=PHI(I)+ALFA*(PHI(I)-THT(I))
0058              CALL WRIT4(PHI,SPI)
0059              S=SPI
0060              IF(IPT.NE.1) GO TO 202
0061              WRITE(IPR,606) (PHI(I),I=1,N)
0062               WRITE(IPR,601) SPI,DEL
0063        202   ICALL=2
            C MAKE EXPL MOVES
0064              GO TO 150
            C IS PRESENT VALUE < BASEPT VALUE
0065        260   IF(S.LT.SSITST) GO TO 200
0066              GO TO 100
            C
            C
            C.....INTERNAL SUBROUTINE TO MAKE EXPLORATIONS ABOUT PHI
0067         150  DO 180 K=1,N
0068              PHIOLD=PHI(K)
0069              STEPK=PHIOLD*.05
0070              IF(STEPK.EQ.0.) STEPK=.05
0071              STEPK=SIGN(STEPK*DEL,XFLG(K))
0072              PHI(K)=PHIOLD+STEPK
0073              CALL WRIT4(PHI,SPI)
0074              IF(IPT.EQ.1) WRITE(IPR,602) ICALL,K,SPI,(PHI(L),L=1,N)
0075              IF(SPI.LT.S) GO TO 179
0076              XFLG(K)=-XFLG(K)
0077              PHI(K)=PHIOLD-STEPK
0078              CALL WRIT4(PHI,SPI)
0079              IF(IPT.EQ.1) WRITE(IPR,602) ICALL,K,SPI,(PHI(L),L=1,N)
0080              IF (SPI.LT.S) GO TO 179
0081              PHI(K)=PHIOLD
0082              GO TO 180
0083         179  S=SPI
0084         180  CONTINUE
0085              GO TO (160,260),ICALL
            C
            C
0086        700   IF (IPT.GE.0) WRITE(IPR,701)
0087        702   DO 703 I=1,N
0088         703  PSI(I)=PHI(I)
0089              IF(IPT.GE.0) WRITE(IPR,607) ITER
0090              RETURN
0091        559   FORMAT(' **** ',I5)
0092        600   FORMAT('  BASE PT:', 1P4(7E15.6,E15.6,/,T9))
0093        606   FORMAT('  PATTERN:', 1P4(7E15.6,E15.6,/,T9))
0094        601   FORMAT(6X,'OBJ:',1PE15.6,5X,'DEL:',E15.6)
0095        602   FORMAT(1X,2I2,' OBJ: ',1PE14.6,'  TRIAL: ',4(6E14.6,E14.6,/,T35))
0096        604   FORMAT('0DEL=',1PE15.6,'     DELMIN=',E15.6,1X,//,
                 *' ITLIM=',I6,'     IPT=',I3)
0097        607   FORMAT(' TOTAL NUMBER OF NEW BASEPOINTS (ITERATIONS) :',I5)
0098        701   FORMAT('0SEARCH TERMINATED BECAUSE NUMBER OF ITERATIONS EXCEEDS LI
                 *MIT.')
0099        704   FORMAT('0SEARCH TERMINATED BECAUSE STEPSIZE LESS THAN LIMIT.')
0100        707   FORMAT('0 STARTING OVER WITH CURRENT BASEPOINT AND INITIAL DEL.')
0101              END
```

Figure B.3 - Computer Code (concluded)